THE GROUP THEORY OF THE HARMONIC OSCILLATOR WITH APPLICATIONS IN PHYSICS

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by

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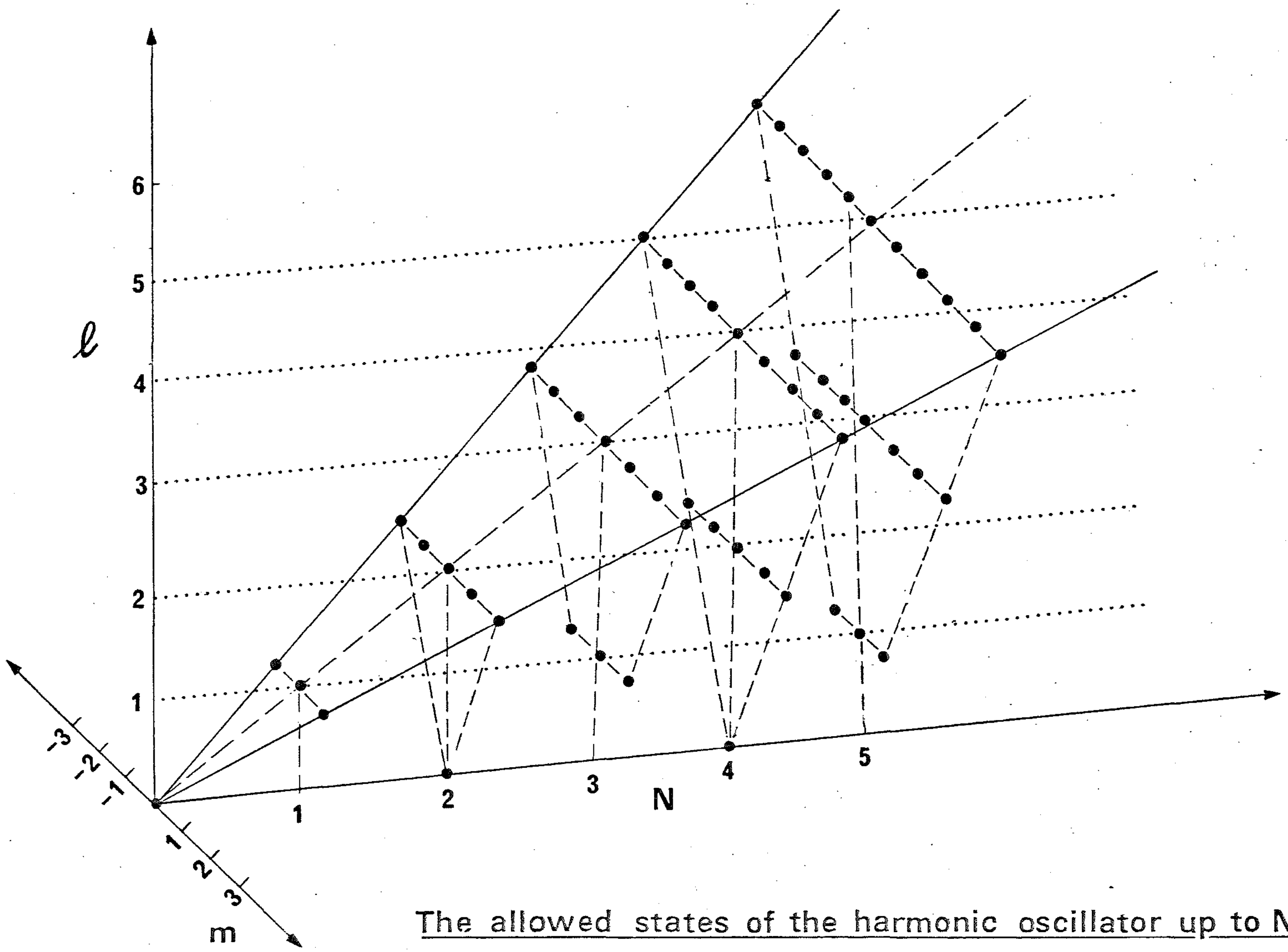

The allowed states of the harmonic oscillator up to N = 5

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Abstract

The possibility of the group SU_3 being used in the description of the $(d+s)^N$ and $(d+s)^n p^m$ many-electron complexes is examined by symmetrization of the Coulomb Hamiltonian. By dividing the Coulomb interaction into symmetry conserving and symmetry violating terms it is found that while the SU_3 scheme tends to give a better description in the $(d+s)^N$ case it shows no improvement over the configurational scheme in the $(d+s)^n p^m$ complex. The scheme is, however, very useful for the calculation of matrix elements of operators normally found in atomic spectroscopy and a complete set of symmetrized , scalar, Hermitian spin-independent two particle operators acting within $(d+s)^n p^m$ configurations is constructed.

The radial wavefunctions of the harmonic oscillator are found to form a basis for the representations of the group O(2,1) in the group scheme $Sp(6,R) \supset SO(3) \times O(2,1)$. The operators $T^k_q = r^{2k}$ are shown to transform simply under the action of the group generators. The matrix elements of T^k_q and a selection rule similar to that of Pasternack and Sternheimer are derived.

Finally the rich group structure of the harmonic oscillator is investigated and a dynamical group proposed which contains, as subgroups, the groups $Sp(6,R)$, $SU(3)$, H_4 and the direct product $O(2,1) \times SO(3)$. Some remarks are made about contractions of groups, semidirect and direct products, and the generalization of the method to n-dimensions.

TABLE OF CONTENTS

INTRODUCTION

This thesis is concerned with the practical applications of the theory of compact and non-compact groups to problems in atomic spectroscopy. The theory of compact groups has been developed by Racah[1] to label n-particle states and to simplify the computation of matrix elements. The application of non-compact groups to physical problems has been developed to a large extent by Barut and it is in this branch of group theory that most of the recent advances are being made. Barut and Kleinert[2] have already shown that the dynamical group of the hydrogen atom is the group O(4,2), and by making use of this group have simplified the solution of the problem an extent unknown before.

The first part of this thesis is concerned with the compact group SU(3) and its application to the theory of the many electron atom. A single particle moving in a three-dimensional harmonic oscillator will give rise to a series of single particle energy levels

1s; 1p; 2s,1d; 2p,1f; 3s,2d,1g; ...

where the levels between successive semi-colons are degenerate in energy. These sets of degenerate levels are associated with solutions of the equation

$$N = 2n+\ell-2$$

where N is a positive integer and n and ℓ are the usual one electron principal and orbital quantum numbers. For a given N the orbital degeneracy is $\frac{(N+1)(N+2)}{2}$ which is just the dimension of the symmetric representation $\{N00\}$ of the group

SU(3). Elliott[3] used this simple observation to construct his SU(3) model for the collective motion of nucleons.

The scheme used is similar to that of Elliott, i.e. $U(2N) \to SU(2) \times [SU(N) \to SU(3) \to R(3)]$. Now it is well known that for a Coulomb field the energy levels depart markedly from those expected for a harmonic oscillator. However, there are frequently quasi-degeneracies such as with the 3d and 4s orbitals in the iron group which lead to a strong mixing in the $(3d+4s)^N$ shell requiring it to be treated as a single entity. The model predicts strong coupling of the ^1D states of $(d+s)^2$, as is indeed observed in Lu(II) by Goldschmidt[4].

In the iron group there is considerable overlapping of the $3d^{N-1}4p$ and $3d^{N-2}4s4p$ configurations which suggests the need for investigating the properties of the $(s+p+d)^N$ configurations. Now $(s+p+d)^N$ involves configurations of both even and odd parity, and it is desirable to work in a scheme having well-defined parity. Schemes investigated are

$$U(8) \to SU(2) \times [SU(4) \to SU(3) \to SO(3)]$$

for the $(s+p)^N$ shell, see Wybourne[5].

$$U(18) \to SU(2) \times [SU(9) \to SU(3) \to SO(3)]$$

for the $(s+p+d)^N$ shell which gives the following linear combination of states.

$$|(30)^1P\rangle = \frac{\sqrt{5}}{3}\,|sp\,^1P\rangle - \frac{2}{3}\,|dp\,^1P\rangle$$

$$|(11)^1P\rangle = \frac{2}{3}\,|sp\,^1P\rangle + \frac{\sqrt{5}}{3}\,|dp\,^1P\rangle$$

This linear combination is found to be roughly in accord with that found by Goldschmidt[4] for the 5d6p + 6s6p configurations of Lu(II). This work is closely related to that of Butler and Wybourne[6] and Chacón[7] for the hydrogen atom. The paper by Moshinsky, Shibuya and Wulfman[8] is especially interesting in that the actual calculations are done in the U(3) basis and then transformed to the R(4) basis of the hydrogen atom. The possibility of using the SU(3) group to simplify calculations in atomic shell theory is also investigated.

The second part of the thesis deals with the theory of non-compact groups and their application to the theory of the harmonic oscillator. Armstrong[9]; Moshinsky, Seligman and Wolf[10]; Moshinsky, Shibuya and Wulfman[8]; Moshinsky and Quesne[11]; Crubellier and Feneuille[13] and Biedenharn and Louck[14] have all treated either the harmonic oscillator explicitly or have treated it implicitly through study of the structure of the groups SU(1,1) or Sp(2,R). In this section the properties of the radial function of the harmonic oscillator is studied using the group scheme $Sp(6,R) \supset SO(3) \times O(2,1)$. The group O(2,1) leads to definition of tensorial properties of $T^k_q = r^{2k}$ for integral and $\frac{1}{2}$ integral k, where r is the radius vector. Coupling coefficients are calculated using Bargmann's[15] method as extended by Cunningham[16] to the group O(2,1). Also a selection rule analogous to that of Pasternack and Sternheimer[17] is derived.

It has been shown by Hwa and Nuyts[12] and Feneuille[13] that the group Sp(6,R) is not the true dynamical group of the harmonic oscillator, as two representations of Sp(6,R) are required to span all of the states of the harmonic oscillator. This observation has led to the use of the semidirect product $H_4 \times)\ Sp(6,R)$ which spans all of the possible states of the harmonic oscillator. The development of this group and its subgroup structure is the subject of the last chapter.

CHAPTER I

APPLICATION OF THE GROUP SU(3) TO THE THEORY OF THE MANY ELECTRON ATOM

I. Introduction

The application of the four-dimensional rotation group R(4) to the interpretation of the degeneracies of the bound states of the hydrogen atom is well known from the early work of Fock[18] and Bargmann[19]. In the non-relativistic hydrogen atom it is found that orbitals having the same principal quantum number, n, are degenerate. However, the dynamical symmetry associated with the hydrogen atom does not persist in many-electron atoms due to the strong symmetry breaking terms arising from the inter-electron Coulomb repulsion studied by Butler[6] and Novaro[20].

Some years ago Racah[21] noted that in the transition series the nd and the (n+1)s orbitals were approximately degenerate with the result that it was necessary to consider the configurations $(s+d)^N$ as a single complex. More recently, Goldschmidt[4] has shown that a similar situation exists in the spectra of the rare earths, her examples of $(5d+6s)^2$ configuration complex of Lu II being of particular relevance here. These observations of approximate degeneracies in many-electron atoms suggest that it may be profitable to investigate the possibility of using symmetry groups other than the group R(4) for many-electron atoms.

The quasi-degeneracy of the nd and (n+1)s orbitals in the transition series suggests that in some cases it could be illuminating to treat the electrons as if they were moving in an isotropic three-dimensional harmonic oscillator potential even though the full n-electron Hamiltonian lacks the necessary SU(3) symmetry.

Some preliminary investigations of the use of harmonic oscillator wavefunctions in atomic problems have been made by Moshinsky[22].

In this thesis the problem of symmetrizing many-electron states according to the transformation group SU(3) is considered and the many-electron Hamiltonian is split into a sum of operators preserving the SU(3) symmetry and operators that break the SU(3) symmetry. These results are then used to explore the validity of interpreting the $(5d+6s)^2$ and (5d+6s)6p complexes of La II and Lu II in terms of SU(3) model wavefunctions. It is found that the configuration mixing in the $(5d+6s)^2$ complex follows approximately that predicted by the SU(3) model while that of the (5d+6s)6p complex is as badly described in the SU(3) model as in the configurational scheme.

II. Infinitesimal Operators of SU(3)

Elliott[3] has shown that the harmonic oscillator Hamiltonian $H_0 = r^2 + b^4p^2$ is not only invariant with respect to the three dimensional operators $L_q = (\underline{r}\times\underline{p})_q$ of R(3) but also to the five components of a second degree tensor operator $Q_q = (\frac{4\pi}{5})^{\frac{1}{2}}\{r^2Y_q^2(\theta_r\varphi_r) + b^4p^2Y_q^2(\theta_p\varphi_p)\}/b^2$ where L_q and Q_q generate the three-dimensional group SU(3). The commutation relations of these operators lead directly to the following results.

$$[L_q,L_{q'}] = -\sqrt{2}\sqrt{3}(-1)^{q+q'}\begin{pmatrix}1 & 1 & 1\\ q & q' & -(q+q')\end{pmatrix}L_{q+q'} \qquad (I.1)$$

$$[Q_q, L_{q'}] = -\sqrt{2}\sqrt{3}\sqrt{5}\ (-1)^{q+q'} \begin{pmatrix} 2 & 1 & 2 \\ q & q' & -(q+q') \end{pmatrix} Q_{q+q'} \qquad (I.2)$$

$$[Q_q, Q_{q'}] = 3\sqrt{2}\sqrt{3}\sqrt{5}\ (-1)^{q+q'} \begin{pmatrix} 2 & 2 & 1 \\ q & q' & -(q+q') \end{pmatrix} L_{q+q'} \qquad (I.3)$$

Now if

$$L_q = \sum_{\ell} A(\ell\ell)\ V_q^{(1)}(\ell\ell) \qquad (I.4)$$

and

$$Q_q = \sum_{\ell\ell'} [B(\ell\ell)V_q^{(2)}(\ell\ell) + C(\ell\ell')\{V_q^{(2)}(\ell\ell') + (-1)^{\ell-\ell'} V_q^{(2)}(\ell'\ell)\}] \qquad (I.5)$$

where $V_q^{(k)}(\ell\ell')$ are the standard tensor operators, see Judd[23]. If L_q and Q_q are to satisfy the commutation relations (I.1,2,3) then $\ell' = \ell+2$ and

$$A(\ell\ell) = \left(\ell(\ell+1)(2\ell+1)/3\right)^{\frac{1}{2}}$$

$$B(\ell\ell) = -(2N+3)\left(\ell(\ell+1)(2\ell+1)/5(2\ell-1)(2\ell+3)\right)^{\frac{1}{2}}$$

$$C(\ell, \ell+2) = \left(6(\ell+1)(\ell+2)(N-\ell)(N+\ell+3)/5(2\ell+3)\right)^{\frac{1}{2}} \qquad (I.6)$$

where the phase convention has been chosen to agree with Elliott and N is the maximal value of ℓ associated with a given harmonic oscillator level. Thus the SU(3) group generators may be written as

$$L_q = \sum_{\ell} \left(\ell(\ell+1)(2\ell+1)/3\right)^{\frac{1}{2}}\ V_q^{(1)}(\ell\ell) \qquad (I.7)$$

$$Q_q = \sum_{\ell} \Bigg[-(2N+3)\ \left\{\frac{(\ell+1)(2\ell+1)}{5(2\ell-1)(2\ell+3)}\right\}^{\frac{1}{2}}\ V_q^{(2)}(\ell\ell) + \left\{\frac{6(\ell+1)(\ell+2)(N-\ell)(N+\ell+3)}{5(2\ell+3)}\right\}^{\frac{1}{2}} \left(V_q^{(2)}(\ell, \ell+2) + V_q^{(2)}(\ell+2, \ell)\right) \qquad (I.8)$$

The summation is over the degenerate shells with ℓ = N, N-2, N-4 ... 1 or 0. For the case of the $(d+s)^N$ complexes ℓ = 2 and

$$L_q = (10)^{\frac{1}{2}} V_q^{(1)}(dd) \tag{I.9}$$

$$Q_q = -[(7)^{\frac{1}{2}} V_q^{(2)}(dd) - 2\{V_q^{(2)}(ds) + V_q^{(2)}(sd)\}]/(15)^{\frac{1}{2}} \tag{I.10}$$

where Q_q has been normalized. To study the $(s+d)^n p^m$ or $(s+p+d)^N$ complexes the following operators are formed.

$$L_q = \sqrt{3}\ \{(10)^{\frac{1}{2}} V_q^{(1)}(dd) + (2)^{\frac{1}{2}} V_q^{(1)}(pp)\}/6 \tag{I.11}$$

$$\begin{aligned} Q_q = \{&-(6)^{\frac{1}{2}} V_q^{(2)}(pp) - (14)^{\frac{1}{2}} V_q^{(2)}(dd) \\ &+ (8)^{\frac{1}{2}}\left(V_q^{(2)}(ds) + V_q^{(2)}(sd)\right)\}/6 \end{aligned} \tag{I.12}$$

III. Group Classification of the $(s+d)^N$ Complex

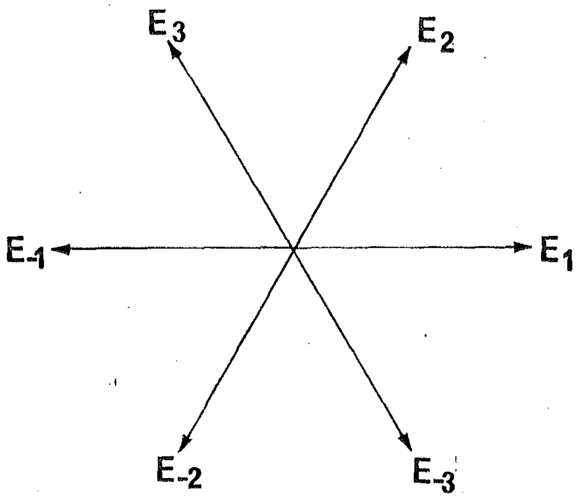
In the case of the $(s+d)^N$ complexes the Weyl self-commuting operators are

$$H_1 = (5)^{\frac{1}{2}} V_0^{(1)}(dd), \qquad H_2 = (5)^{\frac{1}{2}} Q_0 \tag{I.13}$$

and the SU(3) group roots are

$$\begin{aligned} E_1 &= Q_2 \\ E_{-1} &= Q_{-2} \\ E_2 &= \frac{1}{(2)^{\frac{1}{2}}}\ (L_1/(10)^{\frac{1}{2}} + Q_1^2) \\ E_{-2} &= \frac{1}{(2)^{\frac{1}{2}}}\ (L_{-1}/(10)^{\frac{1}{2}} + Q_{-1}^2) \\ E_3 &= \frac{1}{(2)^{\frac{1}{2}}}\ (L_{-1}/(10)^{\frac{1}{2}} - Q_{-1}^2) \\ E_{-3} &= \frac{1}{(2)^{\frac{1}{2}}}\ (L_1/(10)^{\frac{1}{2}} + Q_1^2) \end{aligned} \tag{I.14}$$

lead to the root figure for SU(3)



The root figure for SU(3)

The Casimir operator can easily be constructed and has the form

$$G = 5/6\ (\underset{\sim}{V}^{(1)}(dd)^2 + \underset{\sim}{Q}^{(2)}) \qquad (I.15)$$

with eigenvalues

$$G(\lambda\mu) = \frac{1}{9}\ (\lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu)(\lambda\mu), \qquad (I.16)$$

where $(\lambda\mu)$ denotes a SU(3) representation in Elliott's[3] notation. The irreducible representations of SU(3) are labelled by $(\lambda\mu)$ where $\lambda = f_1 - f_2$ and $\mu = f_2 - f_3$ with the related U(3) representation being labelled by $\{f_1 f_2 f_3\}$. The many-electron states of each $(d+s)^N$ complex may be classified by decomposition of the irreducible representation $\{1^N\}$ of U_{12} under the chain of groups

$$U(12) \rightarrow SU(2) \times [SU(6) \rightarrow SU(3) \rightarrow R(3)] \qquad (I.17)$$

The relevant branching rules may be readily determined by the method of S-function plethysm[24]. Partial tables have been given by Elliott for nuclear problems[3]. The branching rules relevant here are given in table 1. It will be noted that for the $(d+s)^N$ electron complex the classification is almost complete. Elliott has determined the $SU(3) \rightarrow R(3)$ branching rules by noting that the representations D_L of $R(3)$ which occur in the representation $(\lambda\mu)$ of $SU(3)$ are given by

$$L = K,\ K+1,\ K+2\ \ldots\ K+\max\{\lambda\mu\}$$

where the integer $K = \min\{\lambda\mu\}, \min\{\lambda\mu\}-2 \ldots 1$ or 0, with the exception that if $K = 0$ then

$$L = \max\{\lambda\mu\},\ \max\{\lambda\mu\}-2\ \ldots\ 1 \text{ or } 0.$$

The classification of the states of the $(d+s)^N$ complex may be made complete if the orbital states are labelled in the $|(\lambda\mu)KLM_L\rangle$ scheme although in this case the resulting states are not completely orthogonal.

IV. Construction of the SU(3) Symmetrized States

The states of the $(d+s)^N$ complexes may be labelled by the scheme

$$|(d+s)^N(\lambda\mu)KSLM_SM_L\rangle$$

where the quantum numbers M_S and M_L will normally be suppressed. The matrix elements of a scalar two particle operator $G = \sum_{i<j}^{N} g_{ij}$ between any electron complexes χ^N where $\chi = \sum_{i=1}^{N} \ell_i$ may be written as a linear combination of two electron matrix elements in χ^2 weighted by two-particle coefficients of fractional parentage to give[6]

TABLE I

Branching rules for classification of the states of $(d + s)^N$ under $U_{12} \to SU_2 \times (U_6 \to SU_3 \to R_3)$

$U_{12} \to SU_2 \times U_6$	
$\{0\}$	${}^1\{0\}$
$\{1\}$	${}^2\{1\}$
$\{1^2\}$	${}^3\{1^2\} + {}^1\{20\}$
$\{1^3\}$	${}^4\{1^3\} + {}^2\{21\}$
$\{1^4\}$	${}^5\{1^4\} + {}^3\{21^2\} + {}^1\{22\}$
$\{1^5\}$	${}^6\{1^5\} + {}^4\{21^3\} + {}^2\{221\}$
$\{1^6\}$	${}^7\{1^6\} + {}^5\{21^4\} + {}^3\{221^2\} + {}^1\{222\}$

$U_6 \to SU_3$

U_6	SU_3
$\{0\}$	(00)
$\{1\}$	(20)
$\{1^2\}$	(21)
$\{2\}$	(02) (40)
$\{1^3\}$	(03) (30)
$\{21\}$	(11) (22) (41)
$\{1^4\}$	(12)
$\{21^2\}$	(01) (12) (31) (23) (50)
$\{2^2\}$	(20) (31) (04) (42)
$\{1^5\}$	(02)
$\{21^3\}$	(10) (21) (13) (32)
$\{2^21\}$	(02) (21) (13) (40) (32) (24) (51)
$\{1^6\}$	(00)
$\{21^4\}$	(11) (22)
$\{2^21^2\}$	(11) (03) (30) (22) (14) (41) (33)
$\{2^3\}$	(00) (22) (22) (33) (06) (60)

$SU_3 \to R_3$

SU_3	R_3
(00)	S
(10)	P
(11)	PD
(20)	SD
(21)	PDF
(30)	PF
(22)	SD_2FG
(31)	PDFG
(40)	SDG
(32)	PDF_2GH
(41)	PDFGH
(50)	PFH
(51)	PDFGHI
(42)	SD_2FG_2HI
(33)	PDF_2G_2HI
(60)	SDGI

TABLE II

SU_3 symmetrized eigenfunctions of $(d + s)^1$ and $(d + s)^2$

$$|(20)^2S\rangle = |s\ {}^2S\rangle$$
$$|(20)^2D\rangle = |d\ {}^2D\rangle$$

$$|(40)^1G\rangle = |d^2\ {}^1G\rangle$$
$$|(40)^1D\rangle = +\sqrt{\tfrac{7}{9}}\,|ds\ {}^1D\rangle - \sqrt{\tfrac{2}{9}}\,|d^2\ {}^1D\rangle$$
$$|(40)^1S\rangle = \sqrt{\tfrac{5}{9}}\,|s^2\ {}^1S\rangle + \sqrt{\tfrac{4}{9}}\,|d^2\ {}^1S\rangle$$
$$|(02)^1D\rangle = \sqrt{\tfrac{2}{9}}\,|ds\ {}^1D\rangle + \sqrt{\tfrac{7}{9}}\,|d^2\ {}^1D\rangle$$
$$|(02)^1S\rangle = \sqrt{\tfrac{4}{9}}\,|s^2\ {}^1S\rangle - \sqrt{\tfrac{5}{9}}\,|d^2\ {}^1S\rangle$$

$$|(21)^3P\rangle = |d^2\ {}^3P\rangle$$
$$|(21)^3F\rangle = |d^2\ {}^3F\rangle$$
$$|(21)^3D\rangle = |d^2\ {}^3D\rangle$$

$$\langle \chi^N \alpha(\lambda\mu)K;SL|G|\chi^N \alpha'(\lambda'\mu')K';SL\rangle$$

$$= \sum_{\bar{\alpha}(\bar{\lambda}\bar{\mu})\bar{K}\bar{S}\bar{L}} \sum_{(\lambda''\mu'')K''} \sum_{(\lambda'''\mu''')K'''S''L''} (\chi^N \alpha(\lambda\mu)KSL\{|\chi^{N-2}\bar{\alpha}(\bar{\lambda}\bar{\mu})\bar{K}\bar{S}\bar{L};$$

$$(\chi^{N-2}\bar{\alpha}(\bar{\lambda}\bar{\mu})\bar{K}\bar{S}\bar{L};\chi^2(\lambda'''\mu''')S''L'')\langle\chi^2(\lambda''\mu'')K''L''S''|g_{12}|\chi^2(\lambda'''\mu''')K'''S''L''\rangle . \tag{I.18}$$

Observation of this equation shows that SU(3) symmetry can only be conserved in χ^N if the scalar interaction g_{12} is diagonalized in the two electron basis $|\chi^2(\lambda\mu)KSL\rangle$. Thus the usefulness of the group SU(3) as an approximate symmetry may be investigated by consideration of the structure of the χ^2 complex alone.

The states symmetrized according to the scheme $|(d+s)^N(\lambda\mu)KSL\rangle$ may be expanded as a linear combination of the single configuration states. The relevant linear combination may be arrived at by using the fact that the group generator Q cannot couple states belonging to different SU(3) irreducible representations. Since $\langle d^2\ {}^1G| = \langle(40)0\ {}^1G|$ and

$$|(02)0\,{}^1D\rangle = a\,|ds\,{}^1D\rangle + b\,|d^2\ {}^1D\rangle$$

and noting that

$$\langle(40)0\,{}^1G\,|a\,|(02)0\,{}^1D\rangle = 0$$

along with $a^2 + b^2 = 1$ it is found that

$$a = (2)^{\frac{1}{2}}/3 \quad \text{and} \quad b = (7)^{\frac{1}{2}}/3$$

so that finally

$$|(02)0\,{}^1D\rangle = [(2)^{\frac{1}{2}}|ds\,{}^1D\rangle + (7)^{\frac{1}{2}}|d^2\ {}^1D\rangle]/3$$

The complete set of symmetrized states is given in table II.

V. SU(3) Symmetrization of the Coulomb Interaction

To symmetrize the Coulomb interaction with respect to the group SU(3) the one particle tensor operators must be symmetrized with respect to the same chain of groups used to classify the eigenfunctions[6] to give the results of Table III. The Coulomb interaction is then written as

$$H_C = 5F_0(dd)\varepsilon_0 + 14F_2(dd)\varepsilon_2 + 70F_4(dd)\varepsilon_4 + F_0(ss)\varepsilon_5$$
$$+ F_0(ds)\varepsilon_6 + 2G_2(ds)\varepsilon_7 + 2(5)^{\frac{1}{2}} H_2(ds)\varepsilon_9 \qquad (I.19)$$

where the ε_k's are two particle operators as defined in Table IV and their coefficients are the usual Slater radial integrals.

The Coulomb interaction is then rewritten as

$$H_C = \sum_{K=0}^{9} e_k E_k \qquad (I.20)$$

where the e_k's are linear combinations of the ε_k's of Table IV having well defined SU(3) symmetry. The appropriate linear combinations are given in Table V while Table VI gives the expansion of the E_k's as linear combinations of the Slater radial integrals. These linear combinations are then determined by well known standard methods. The operators e_0, e_1 and e_2 are all scalars in SU(3) and thus conserve the SU(3) symmetry while the remaining e_k's can couple different SU(3) irreducible representations and thus constitute symmetry breaking terms.

The matrix elements of the e_k's may be calculated directly in the SU(3) scheme for the case of (00) symmetry as these are diagonal in the SU(3) labels.

TABLE III

Symmetrization of one-particle tensor operators for $(d+s)^N$

U_{12}	$SU_2 \times U_6$	$SU_2 \times SU_3$	$SU_2 \times R_3$	Symmetrized operator
$\{21^{10}\}$	$^1\{21^4\}$	$^1(11)$	^1P	$V^{(1)}(dd)$
			^1D	$(1/\sqrt{15})[-\sqrt{7}V^{(2)}(dd) + \sqrt{8}\,{}^+V^{(2)}(ds)]$
		$^1(22)$	^1S	$(1/\sqrt{6})[-\sqrt{5}V^{(0)}(ss) + V^{(0)}(dd)]$
			$^1D_0$	$(1/\sqrt{15})[\sqrt{8}\,V^{(2)}(dd) + \sqrt{7}\,{}^+V^{(2)}(ds)]$
			^1F	$V^{(3)}(dd)$
			^1G	$V^{(4)}(dd)$
			$^1D_2$	$\bar{V}^{(2)}(ds)$
		$^3(11)$	^3P	$V^{(1)}(dd)$
			^3D	$(1/\sqrt{15})[\sqrt{7}V^{(2)}(dd) + \sqrt{8}\,{}^+V^{(2)}(ds)]$
		$^3(22)$	^3S	$(1/\sqrt{6})[-\sqrt{5}V^{(0)}(ss) + V^{(0)}(dd)]$
			$^3D_0$	$(1/\sqrt{15})[\sqrt{8}V^{(2)}(dd) + \sqrt{7}\,{}^+V^{(2)}(ds)]$
			^3F	$V^{(3)}(dd)$
			^3G	$V^{(4)}(dd)$, $^3D_2$, $\bar{V}^{(2)}(ds)$
$\{0\}$	$\{0\}$	$^1(00)$	^1S	$(1/\sqrt{6})[V^{(0)}(ss) + \sqrt{5}V^{(0)}(dd)]$

TABLE IV

R₃ symmetrized operators

$$\varepsilon_0 = \sum_{i>j} V_i^{(0)}(dd)\cdot V_j^{(0)}(dd)$$

$$\varepsilon_1 = \sum_{i>j} V_i^{(1)}(dd)\cdot V_j^{(1)}(dd)$$

$$\varepsilon_2 = \sum_{i>j} V_i^{(2)}(dd)\cdot V_j^{(2)}(dd)$$

$$\varepsilon_3 = \sum_{i>j} V_i^{(3)}(dd)\cdot V_j^{(3)}(dd)$$

$$\varepsilon_4 = \sum_{i>j} V_i^{(4)}(dd)\cdot V_j^{(3)}(dd)$$

$$\varepsilon_5 = \sum_{i>j} V_i^{(0)}(ss)\cdot V_j^{(0)}(ss)$$

$$\varepsilon_6 = \sqrt{5}\sum_{i>j} [V_j^{(0)}(ss)\cdot V_j^{(0)}(dd) - V_i^{(0)}(dd)\cdot V_j^{(0)}(ss)]$$

$$\varepsilon_7 = \sum_{i>j} {}^+V_i^{(2)}(ds)\cdot {}^+V_j^{(2)}(ds)$$

$$\varepsilon_8 = \sum_{i>j} {}^-V_i^{(2)}(ds)\cdot V_j^{(2)}(ds)$$

$$\varepsilon_9 = \sqrt{14}\sum_{i>j} [V_i^{(2)}(dd)\cdot {}^+V_j^{(2)}(ds) + {}^+V_i^{(2)}(ds)\cdot V_j^{(2)}(dd)]$$

TABLE V

The SU_3 symmetrized e_k operators

SU_3	Normalization	e_k
(00)	$\frac{1}{6}$	$e_0 = 5\varepsilon_0 + \varepsilon_5 + \varepsilon_6$
(00)	$(2)^{\frac{1}{2}}/60$	$e_1 = 15\varepsilon_1 + 7\varepsilon_2 + 8\varepsilon_7 - 2\varepsilon_9$
(00)	$(3)^{\frac{1}{2}}/270$	$e_2 = -5\varepsilon_0 - 16\varepsilon_2 - 30\varepsilon_3 - 30\varepsilon_4 - 25\varepsilon_5 + 5\varepsilon_6 - 14\varepsilon_7 + 30\varepsilon_8 - 4\varepsilon_9$
(22)	$(5)^{\frac{1}{2}}/15$	$e_3 = 5\varepsilon_0 - 5\varepsilon_5 - 2\varepsilon_6$
(22)	$(3)^{\frac{1}{2}}/30$	$e_4 = -25\varepsilon_1 + 7\varepsilon_2 + 8\varepsilon_7 - 2\varepsilon_9$
(22)	$(70)^{\frac{1}{2}}/1050$	$e_5 = 56\varepsilon_2 - 56\varepsilon_7 - \varepsilon_9$
(22)	$(30)^{\frac{1}{2}}/1800$	$e_6 = 20\varepsilon_0 - 32\varepsilon_2 - 75\varepsilon_3 + 45\varepsilon_4 + 100\varepsilon_5 - 20\varepsilon_6 - 28\varepsilon_7 - 60\varepsilon_8 - 8\varepsilon_9$
(22)	$(42)^{\frac{1}{2}}/2520$	$e_7 = 28\varepsilon_0 + 32\varepsilon_2 - 15\varepsilon_3 - 87\varepsilon_4 + 140\varepsilon_5 - 28\varepsilon_6 + 28\varepsilon_7 - 84\varepsilon_8 + 8\varepsilon_9$
(44)	$(70)^{\frac{1}{2}}/1260$	$e_8 = 14\varepsilon_0 + 16\varepsilon_2 - 15\varepsilon_3 + 9\varepsilon_4 + 70\varepsilon_5 - 14\varepsilon_6 + 14\varepsilon_7 + 42\varepsilon_8 - 4\varepsilon_9$
(60) + (06)	$(3410)^{\frac{1}{2}}/17050$	$e_9 = 28\varepsilon_0 - 40\varepsilon_2 + 60\varepsilon_3 - 12\varepsilon_4 + 140\varepsilon_5 - 28\varepsilon_6 - 35\varepsilon_7 + 21\varepsilon_8 - 10\varepsilon_9$

TABLE VI

Radial coefficients for SU_3 symmetry

$$E_0 = \tfrac{1}{6}\,[25F_0(dd) + F_0(ss) + 10F_0(ds)]$$

$$E_1 = (\sqrt{2}/12)[98F_2(dd) + 16G_2(ds) - 56\sqrt{(10)}\,H_2(ds)]$$

$$E_2 = (\sqrt{3}/54)[-5F_0(dd) - 224F_2(dd) - 3780F_4(dd) - 5F_0(ss) + 10F_0(ds) - 28G_2(ds) - \sqrt{(10)}\,112H_2(ds)]$$

$$E_3 = (\sqrt{5}/30)[25F_0(dd) - 5F_0(ss) - 20F_0(ds)]$$

$$E_4 = (\sqrt{3}/60)[98F_2(dd) + 16G_2(ds) - 56\sqrt{(10)}\,H_2(ds)]$$

$$E_5 = (\sqrt{(70)}/420)[784F_2(dd) - 112G_2(ds) - 28\sqrt{(10)}\,H_2(ds)]$$

$$E_6 = (\sqrt{(30)}/360)[20F_0(dd) - 448F_2(dd) + 5670F_4(dd) + 20F_0(ss) - 40F_0(ds) - 56G_2(ds) - 224\sqrt{(10)}\,H_2(ds)]$$

$$E_7 = (\sqrt{(42)}/2520)[140F_0(dd) + 2240F_2(dd) - 54810F_4(dd) + 140F_0(ss) - 280F_0(ds) + 280G_2(ds) + 1120\sqrt{(10)}\,H_2(ds)]$$

$$E_8 = (\sqrt{5}/180)[70F_0(dd) + 1120F_2(dd) + 5670F_4(dd) + 70F_0(ss) - 140F_0(ds) + 140G_2(ds) + 500\sqrt{(10)}\,H_2(ds)]$$

$$E_9 = (\sqrt{(3410)}/17050)[140F_0(dd) - 2800F_2(dd) - 7560F_4(dd) + 140F_0(ss) - 280F_0(ds) - 350G_2(ds) - 1400\sqrt{(10)}\,H_2(ds)]$$

TABLE VIII

Calculated values of the SU_3 radial integrals for the $(5d + 6s)^2$ complex of La II in cm^{-1}

$E_0 = 31561$	$E_1 = 1278$	$E_2 = -14144$
$E_3 = 285$	$E_4 = 310$	$E_5 = 2921$
$E_6 = -5121$	$E_7 = 4440$	$E_8 = 2482$
	$E_9 = -10415$	

The matrix elements of the operator

$$e_0 = (5\varepsilon_0 + \varepsilon_5 + \varepsilon_6)/6$$

are readily found to be just N(N-1)/12. Now the Casimir operator G of SU(3) has the form

$$G = \frac{5}{6} (\underline{V}^1(dd)^2 + \underline{Q}^2) \tag{I.21}$$

with eigenvalues

$$g = (\lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu) \tag{I.22}$$

This result may be used to calculate the matrix elements of the operators e_1 and e_2 giving the results

$$\langle (d+s)^N(\lambda\mu)SL|e_1|(d+s)^N(\lambda'\mu')SL\rangle$$

$$= \frac{\sqrt{2}}{60} (9g - 10N)\delta_{\lambda\lambda'}\delta_{\mu\mu'} \tag{I.23}$$

and

$$\langle (d+s)^N(\lambda\mu)SL|e_2|(d+s)^N(\lambda'\mu')SL\rangle =$$

$$\frac{\sqrt{3}}{540} (36g + 60S(S+1) + 5N(4N-21))\delta_{\lambda\lambda'}\delta_{\mu\mu'} \tag{I.24}$$

where S is the spin of the state.

The calculation of the matrix elements of $e_3, e_4, \ldots, e_9$ is, even with the help of SU(3) Clebsch-Gordon coefficients, a more tedious task, but a list of them for the $(d+s)^N$ complex appears in Table VII. The Coulomb interaction may now be split into the SU(3) symmetry preserving part $e_0E_0 + e_1E_1 + e_2E_2$ and the symmetry breaking part $(e_3E_3 + e_4E_4 + e_5E_5 + e_6E_6 + e_7E_7 + e_8E_8 + e_9E_9)$. The SU(3) model will be valid only if the latter part is small compared to the former. The values of E_k for the $(5d+6s)^2$ complex of La II are given in Table VIII. These values were calculated using the empirical values of the Slater integrals found by Goldschmidt.

TABLE VII

Matrix elements of the SU_3 e_k operators in the $(d+s)^2$ complex

	e_0	e_1	e_2	e_3	e_4	e_5	e_6	e_7	e_8	e_9
$\langle(40)^1G\,\lvert e_k\rvert\,(40)^1G\rangle$	1	8	−9	1	−8	16	−12	15	6	0
$\langle(40)^1D\,\lvert e_k\rvert\,(40)^1D\rangle$	1	8	−9	$-\frac{4}{3}$	$\frac{32}{3}$	$-\frac{64}{9}$	16	−16	−36	0
$\langle(40)^1S\,\lvert e_k\rvert\,(40)^1S\rangle$	1	8	−9	$-\frac{7}{3}$	$\frac{59}{3}$	6	28	28	126	0
$\langle(02)^1S\,\lvert e_k\rvert\,(02)^1S\rangle$	1	−10	−45	$-\frac{5}{3}$	$\frac{10}{3}$	10	230	70	0	0
$\langle(02)^1D\,\lvert e_k\rvert\,(02)^1D\rangle$	1	−10	−45	$-\frac{1}{3}$	$-\frac{2}{3}$	$-\frac{56}{3}$	−46	−14	0	0
$\langle(02)^1S\,\lvert e_k\rvert\,(40)^1S\rangle$	0	0	0	$-\frac{4}{3}\sqrt{5}$	$\frac{40}{9}\sqrt{5}$	$-\frac{4}{9}\sqrt{5}$	$-8\sqrt{5}$	$56\sqrt{5}$	0	$63\sqrt{5}$
$\langle(02)^1D\,\lvert e_k\rvert\,(40)^1D\rangle$	0	0	0	$-\frac{1}{3}\sqrt{(14)}$	0	$-5\sqrt{(14)}$	$-2\sqrt{(14)}$	$14\sqrt{(14)}$	0	$18\sqrt{(14)}$
$\langle(21)^3P\,\lvert e_k\rvert\,(21)^3P\rangle$	1	−4	27	1	−9	28	−64	126	0	0
$\langle(21)^3D\,\lvert e_k\rvert\,(21)^3D\rangle$	1	−4	27	2	4	28	−36	0	0	0
$\langle(21)^3F\lvert e_k\rvert(21)^3F\rangle$	1	−4	27	1	−1	−32	54	6	0	0
Normalization of operator	$\frac{1}{6}$	$\frac{\sqrt{2}}{60}$	$\frac{\sqrt{3}}{270}$	$\frac{\sqrt{5}}{15}$	$\frac{\sqrt{3}}{30}$	$\frac{\sqrt{(70)}}{1050}$	$\frac{\sqrt{(30)}}{1800}$	$\frac{\sqrt{(42)}}{2520}$	$\frac{\sqrt{(70)}}{1260}$	$\frac{\sqrt{(3410)}}{17050}$

VI. SU(3) and the $(5d+6s)^2$ Complex of LaII

The values of the E_k's given in Table VIII may be used with the e_k's given in Table VII to yield the Coulomb matrix elements for the $(5d+6s)^2$ complex of LaII. Upon diagonalizing the two-by-two matrices associated with the ^1S and ^1D states it is found that the lowest energy states may be written as

$$|^1S\rangle = 0.927|(40)^1S\rangle + 0.376|(02)^1S\rangle$$

$$= 0.942|6s^2\ ^1S\rangle + 0.337|5d^2\ ^1S\rangle$$

and

$$|^1D\rangle = 0.987|(02)^1D\rangle + 0.179|(40)^1D\rangle$$

$$= 0.622|5d6s\ ^1D\rangle + 0.783|5d^2\ ^1D\rangle$$

It is at once apparent that the ^1D states follow the SU(3) model very closely and indeed the SU(3) scheme is superior to that of the usual configurational scheme while for the ^1S states the configurational scheme is marginally better. It should be noted here that the spin orbit interaction has been ignored here as in the case of singlet states it is of second order. The principal contribution to the SU(3) symmetry breaking term is the term e_9E_9 which has off-diagonal elements that strongly mix the (02) and (40) representations at SU(3).

VII. The SU(3) Model and the $(d+s)^m p^n$ Complex

The states of the $(d+s)^m p^n$ complex form a subset of the states of the $(s+p+d)^{m+n}$ complex which span the $\{1^{m+n}\}$ irreducible representation of U(18). The states of the latter complex may be classified under the chain of groups

$$U(18) \rightarrow SU(2) \times [U(9) \rightarrow SU(3) \rightarrow R(3)] \qquad (I.25)$$

to give the classification for $m+n \leqslant 2$ as shown in Table IX.

The states of $(d+s)p$ may be symmetrized according to the different irreducible representations of SU(3) to give the results of Table X. Only the ^3P and ^1P states will have off-diagonal Coulomb matrix elements. Upon using the empirical radial integrals given by Goldschmidt for the $(5d+6s)6p$ complex of Lu II and then diagonalizing the two-by-two Coulomb matrices it is found that the eigenfunctions for the lowest ^3P and ^1P states are:

$$|^3P\rangle = 0.852|5d6p\ ^3P\rangle + 0.523|6s6p\ ^3P\rangle$$

$$= 0.847|(11)^3P\rangle + 0.532|(30)^3P\rangle$$

and

$$|^1P\rangle = 0.838|5d6p\ ^1P\rangle + 0.547|6s6p\ ^1P\rangle$$

$$= 0.836|(11)^1P\rangle + 0.548|(30)^1P\rangle.$$

It is clear in this case that neither the configurational or SU(3) scheme gives a satisfactory model.

VIII. Conclusion

While the SU(3) scheme appears to give a better description of the $(d+s)^N$ complex compared to that of the single configuration schemes it is of no real advantage in dealing with the $(d+s)^m p^n$ complexes. In the latter situation neither scheme is a realistic approximation to the physical situation. The destruction of the SU(3) scheme comes from the large symmetry breaking terms in $\sum_{i<j} e^2/r_{ij}$ and the results found for $(d+s)^N$ must be regarded as somewhat

TABLE IX

Classification of the states of $(d + s)^m p^n$ for $m + n \leq 2$

U_{18}	$SU_2 \times U_9$	$SU_2 \times SU_3$	^{2S+1}L	Configurations
{0}	$^1\{0\}$	$^1(00)$	^1S	—
{1}	$^2\{1\}$	$^2(10$	^2P	p
		$^2(20)$	^2SD	d + s
$\{1^2\}$	$^3\{1^2\}$	$^3(01)$	^3P	p^2
		$^3(11)$	^3PD	(d + s)p
		$^3(30)$	^3PF	(d + s)p
		$^3(21)$	^3PDF	$(d + s)^2$
	$^1\{2\}$	$^1(20)$	^1SD	p^2
		$^1(11)$	^1PD	(d + s)p
		$^1(30)$	^1PF	(d + s)p
		$^1(02)$	^1SD	$(d + s)^2$
		$^1(40)$	^1SDG	$(d + s)^2$

TABLE X

SU_3 Symmetrized states of the (d + s)p complex

$$|(11)^3P\rangle = \tfrac{2}{3}\,|sp\;^3P\rangle + \tfrac{1}{3}(5)^{\frac{1}{2}}\,|dp\;^3P\rangle$$
$$|(30)^3P\rangle = \tfrac{1}{3}(5)^{\frac{1}{2}}\,|sp\;^3P\rangle - \tfrac{2}{3}\,|dp\;^3P\rangle$$
$$|(30)^3F\rangle = |dp\;^3F\rangle$$
$$|(11)^3D\rangle = |dp\;^3D\rangle$$
$$|(11)^1P\rangle = \tfrac{2}{3}\,|sp\;^1P\rangle + \tfrac{1}{3}(5)^{\frac{1}{2}}\,|dp\;^1P\rangle$$
$$|(30)^1P\rangle = \tfrac{1}{3}(5)^{\frac{1}{2}}\,|sp\;^1P\rangle - \tfrac{2}{3}\,|dp\;^1P\rangle$$
$$|(11)^1D\rangle = |dp\;^1D\rangle$$
$$|(30)^1F\rangle = |dp\;^1F\rangle$$

fortuitous. This result, taken with earlier work on the application of R(6) and R(4) to the $(s+d)^N$ and $(s+p)^N$ complexes shows that even for these relatively simple cases compact groups are not good approximations to the physical situation. Finally even though SU(3) does not appear to be a good approximation to the physical scheme it does supply a useful classification scheme for otherwise incompletely labelled states and thus may be used to obviate the calculation at certain spectroscopic quantities, this use for SU(3) will be studied in the next chapter.

CHAPTER II

STUDY OF THE ONE AND TWO PARTICLE OPERATORS ASSOCIATED WITH THE GROUP SU(3) AND THE $(d+s)^n p^m$ CONFIGURATIONS

I. Introduction

The whole of this chapter was written in conjunction with A. Crubellier and S. Feneuille of Laboratoire Aime Cotton, C.N.R.S. II, Orsay, Essonne, France, and was presented in a similar form to LA THEORIE DE LA STRUCTURE ATOMIQUE, GIF-SUR-YVETTE, 8-11 July 1970.

In this chapter the properties of the one and two electron operators first noticed in chapter one are considerably extended, and their usefulness in calculating matrix elements of various spectroscopic coefficients is shown. Following the work of Elliott[3] numerous studies of mixed configurations have been made[4,25,26]. They have all been characterized by the use of a multiconfigurational model, i.e. all the configurations $\ell_1^{n_1}\ \ell_2^{n_2}\ \ell_3^{n_3} \ldots \ell_r^{n_r}$ where $\sum_{i=1}^{r} n_i = N$ are treated simultaneously. Usually the collection of configurations $(\sum_{i=1}^{r} \ell_i)^N$ is considered, however with the exception of the very specialized cases of hydrogenic and harmonic oscillator potentials, this simultaneous treatment is only justifiable for the $(d+s)^N$ configurations of the transition elements which have already been studied in great detail[27,28,29,30,31]. It seems unreasonable to include in the treatment of the odd configurations $(d+s)^{N-1}p$ of the transition elements, the configurations $(d+s)^{N-2}p^2$, $(d+s)^{N-3}p^3$ etc. as the configuration interactions thus taken into account are quite small.

In this chapter it will be shown that using the work of Elliott[3] as a basis, the configurations under study can be characterized by the scheme

$|(d+s)^n\ S_1\{\lambda_1\},\ P^m S_2\{\lambda_2\} k\ SL\ J\ M_J>$ where $\{\lambda_1\}$ and $\{\lambda_2\}$ are irreducible representations of the group SU(3) and k is a supplementary quantum number required to characterize the states completely as noted in chapter one. According to the choice of generators in the different group structures, two distinct classifications can be developed, but it is shown that for some configurations neither one nor the other leads to states (of configurational mixing) near those obtained by parametric methods, and furthermore that any unmixed coupling is not explained in a satisfactory fashion especially for the heavy elements of the transition series. However, the bases thus defined have several advantages because of their well-defined symmetry properties. In order to use these symmetry properties, the properties of the single electron operators for interaction between d, s and p electrons, are alotted wholely to one of the two proposed classifications. The group of scalar, symmetric, Hermitian two particle operators independent of spin acting within the configurations is constructed within the $(d+s)^m p^n$ configurations and turns out to possess well defined transformation properties belonging to the chain of groups under consideration.

II. Classification of the $(d+s)^m p^n$ Configuration States

Under the scheme of Elliott[3] the states of the configuration $(d+s)^m p^n$ are described by their transformation properties under the operations of the different groups in the following chain.

$$SU(2)(d,s) \times [\overset{\varepsilon\varepsilon'}{SU}(6)(d,s) \supset \overset{\varepsilon\varepsilon'}{SU}(3)(d,s) \supset R_3(d,s)]$$

This chain of groups allows the formation of the following types of operators

$$SU(2)(d,s) \; : \; (6)^{-\frac{1}{2}}[(5)^{\frac{1}{2}}\underline{W}^{10}(d,d) + \underline{W}^{10}(s,s)]$$

$$\overset{\varepsilon\varepsilon'}{SU}(6)(d,s) \; : \; \underline{V}^1(d,d),\ \varepsilon\underline{V}^2(d,d),\ \underline{V}^3(d,d),\ \varepsilon^1\underline{V}^2(d,s),$$

$$\varepsilon^1\underline{V}^2(s,d),\ (6)^{-\frac{1}{2}}[(5)^{\frac{1}{2}}\underline{V}^0(s,s) - \underline{V}^0(d,d)].$$

$$\overset{\varepsilon\varepsilon'}{SU}(3) \; : \; \underline{V}^1(d,d),\ \underline{V}^{+2}(\varepsilon\varepsilon') = (15)^{-\frac{1}{2}}[\varepsilon(7)^{\frac{1}{2}}\underline{V}^2(d,d)$$

$$+ \varepsilon^1 2\{\underline{V}^2(d,s) + \underline{V}^2(s,d)\}]$$

$$R_3(d,s) \; : \; \underline{V}^1(d,d)$$

In these expressions ε and ε' can take values ± 1, the operators $W^{(K'K)}(\ell_a\ell_b)$ and $V^k(\ell_a\ell_b) = (2)^{\frac{1}{2}}W^{(0k)}(\ell_a\ell_b)$ are defined in reference 25. In addition the states of a p^m configuration can be classified by their symmetry properties under the classical chain

$$SU(2)(p) \times [\overset{\varepsilon''}{SU}(3)(p) \supset R_3(p)]$$

where the generators of the different groups are

$$SU(2)(p) \; : \; \underline{W}^{10}(pp)$$

$$\overset{\varepsilon''}{SU}(3)(p) \; : \; \underline{V}^1(pp),\ \varepsilon''\underline{V}^2(pp)$$

$$R_3(p) \; : \; \underline{V}^1(pp)$$

The states of a $(d+s)^m p^n$ configuration can be classified with the aid of the following chain which has already been used by Flores and Moshinsky[32]

$$[SU(2)(d,s) \times SU(2)(p) \supset SU(2)] \times \{[\overset{\varepsilon'}{SU(6)}(d,s) \supset \overset{\varepsilon\varepsilon'}{SU(3)}(d,s)]$$

$$\times\ SU(3)(p) \supset R_3(d,s) \times R_3(p) \supset R_3\}.$$

Where the direct product should be emphasized, this chain does not give any more information beyond that introduced by previous chains. However the following reduction can also be made.

$$\overset{\varepsilon\varepsilon'}{SU(3)}(d,s) \times \overset{\varepsilon''}{SU(3)}(p) \supset SU(3) \supset R(3)$$

where the group SU(3) is defined by the following generators

$$\underline{V}^{(1)} = (6)^{-\frac{1}{2}}[(5)^{\frac{1}{2}}\underline{V}^1(dd) + \underline{V}^1(pp)]$$

$$\underline{V}^{(2)} = (6)^{-\frac{1}{2}}[(5)^{\frac{1}{2}}\underline{V}^{+2}(\varepsilon\varepsilon') + \varepsilon''\underline{V}^2(pp)].$$

There is a definite gain here because a new group appears, which is not the direct product of the two groups associated with the d,s and p electrons. With regard to the quantum numbers introduced it would appear, _a priore_, necessary to characterize the configuration states studied by an irreducible representation of each of the groups of the chosen chain; S_1 for SU(2)(p), $\{\lambda_2\}$ for $\overset{\varepsilon''}{SU(3)}(p)$, $\{\lambda\}$ for SU(3), S for SU(2) and L for R(3). However, it can be easily seen that the representations $\{\mu\}$ and $\{\lambda_2\}$ are equal to,

$$\left\{2^{(3 - \varepsilon(3-n/2) - S_1)},\ 1^{2S_1}\right\}$$

and

$$\left\{2^{(\frac{3}{2} - \varepsilon''(\frac{3}{2} - \frac{m}{2}) - S_2)},\ 1^{2S_2}\right\}$$

(where $\{\mu\}$ is for $\overset{\varepsilon\varepsilon'}{SU(6)}(d,s)$)

respectively[25] and the listing of these representations is superfluous once the values of ε, ε'', n, m and S_1 and S_2 have been specified. In the scheme adopted a given state is written as follows.

$$|\varepsilon\varepsilon'(d+s)^n S_1\{\lambda_1\},\varepsilon'' p^m S_2,\{\lambda\} SL\ J\ M_J\rangle$$

Now a difficulty arises, already mentioned in chapter one, namely the appearance of multiple L values in the reduction of the SU(3) representations $\{\lambda\}$. Also multiplicities may also occur in the reduction of $\{\mu\}$ to a sum of $\{\lambda_1\}$. Thus the proposed classification is not complete and a supplementary quantum number, k, must be added to completely characterize the states.

Now at first inspection it would appear that for given values of ε, ε' and ε'' eight distinct classification schemes can be obtained, but note that the choice of $\varepsilon' = \pm 1$ is really equivalent to choosing the relative phase of the single electron (d+s) state and is thus of no physical significance, moreover the two classifications $(\varepsilon,\varepsilon',\varepsilon'')$ and $(-\varepsilon,-\varepsilon',-\varepsilon'')$ are equivalent, since the second can be deduced immediately from the first by use of the relation:

$$(\sigma_1\sigma_2)(\sigma_3\sigma_4) = \Sigma\ g(\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6)(\sigma_5\sigma_6)$$

which implies

$$(\sigma_2\sigma_1)(\sigma_4\sigma_3) = \Sigma\ g(\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6)(\sigma_5\sigma_6)$$

which itself arises from the hole-particle equivalence for d and s electrons, which in this case takes the form

$$\left\{2^{(\frac{n}{2}-S_1)},\ 1^{2S_1}\right\} = \Sigma\ g(n,S_1,\sigma_1\sigma_2)(\sigma_1\sigma_2)$$

$$\left\{2^{(6-\frac{n}{2}-S_1)},\ 1^{2S_1}\right\} = \Sigma\ g(n,S_1,\sigma_1\sigma_2)(\sigma_1\sigma_2).$$

where $(\sigma_1\sigma_2)$ represents a state in SU(3). Hence finally only the product $\varepsilon\varepsilon''$ is of physical significance. The (d+s)p configuration states for the two possible cases $\varepsilon\varepsilon'' = \pm 1$ and the projection of the dp and sp configuration states are listed in Table I. Hence the results of Table II can be obtained in the decomposition of the representations

$$\left\{2^{(\frac{n}{2}-S_1)},\ 1^{2S_1}\right\}$$

for $n \leqslant 6$ in the reduction $\overset{+\varepsilon'}{SU(6)}(d,s) \supset \overset{+\varepsilon'}{SU(3)}(d,s)$ and if $n \geqslant 6$ or $\varepsilon = -1$ the hole-particle equivalence mentioned above can be used. The reduction of $SU(3) \times SU(3) \supset SU(3)$ is obtained directly from Littlewood's rules[33] and the rules for reducing SU(3) to R(3) are given in chapter one.

III. Development of Some Physical States on the Proposed Bases

The first problem which arises is to find whether the states of one of the two classifications proposed are sufficiently close to the states actually occurring in the (d+s)p configurations of the transition elements.

In order to see if this is so, some particular cases of the Coulomb interaction and spin orbit coupling matrices have been diagonalized in each of the two bases, assigning to the Slater integrals and the spin-orbit coupling constraints values which have been obtained in previous studies by parametric means. The specific examples considered were some of the fairly heavy elements since for these simultaneous

TABLE I

Decomposition of the representations $\left\{2^{\frac{n}{2}-S_1},\ 1^{2S_1}\right\}$, $n \leqslant 6$ of SU(6)(d,s) in the reduction SU(6)(d,s) $\supset$ SU(3)(d,s)

SU(6)(d,s) n	S_1	SU(3)(d,s)
-	-	-
0	0	(00)
1	$\frac{1}{2}$	(20)
2	0	(02) (40)
2	1	(21)
3	$\frac{1}{2}$	(11) (22) (41)
3	$\frac{3}{2}$	(03) (30)
4	0	(20) (31) (04) (42)
4	1	(01) (12) (31) (23) (50)
4	2	(12)
5	$\frac{1}{2}$	(02) (21) (13) (40) (32) (24) (51
5	$\frac{3}{2}$	(10) (21) (13) (32)
5	$\frac{5}{2}$	(02)
6	0	(00) (22) (22) (33) (06) (60)
6	1	(11) (03) (30) (22) (14) (41) (33
6	2	(11) (22)
6	3	(00)

TABLE II

(d+s)p configuration states in the proposed classifications

$\varepsilon\varepsilon'' = 1$

$$|^{1,3}(11)P\rangle = \tfrac{1}{3}[-\varepsilon(5)^{\frac{1}{2}}|dp\,^{1,3}P\rangle + 2\varepsilon'\,|sp\,^{1,3}P\rangle$$

$$|^{1,3}(11)D\rangle = |dp\,^{1,3}D\rangle$$

$$|^{1,3}(30)P\rangle = \tfrac{1}{3}[2\varepsilon|dp\,^{1,3}P\rangle + (5)^{\frac{1}{2}}\varepsilon'\,|sp\,^{1,3}P\rangle$$

$$|^{1,3}(30)F\rangle = |dp\,^{1,3}F\rangle$$

$\varepsilon\varepsilon'' = -1$

$$|^{1,3}(10)P\rangle = \frac{1}{(6)^{\frac{1}{2}}}\,[\varepsilon(5)^{\frac{1}{2}}|dp\,^{1,3}P\rangle + \varepsilon'\,|sp\,^{1,3}P\rangle$$

$$|^{1,3}(21)P\rangle = \frac{1}{(6)^{\frac{1}{2}}}\,[-\varepsilon|dp\,^{1,3}P\rangle + \varepsilon'\,|sp\,^{1,3}P\rangle$$

$$|^{1,3}(21)D\rangle = |dp\,^{1,3}D\rangle$$

$$|^{1,3}(21)F\rangle = |dp\,^{1,3}F\rangle$$

treatment of the d^np, $d^{n-1}sp$ and $d^{n-2}s^2p$ configurations is clearly justified and there are corresponding parametric studies available[4, 34].

The two configurations studied were the $(5d+6s)6p$ configuration of Lu II and the $(5d+6s)^26p$ one of Hf II. The results are summarized in Tables III and IV, under different J values. The results are listed according to the mean coupling (defined as the mean of the square of the biggest components) in the two bases under consideration. By way of comparison the mean coupling obtained in the bases due to Racah which is defined as follows:

$$|d^nV_1SL_1,P,SL\rangle, \quad |d^{n-1}\overline{V}\,\overline{S}\,\overline{L},S,S_1L_1,P,SL\rangle,$$

$$|d^{n-2}s^2\overline{V}_1S_1L_1,P,SL\rangle,$$

and also the L-S coupling which is a measure of relative importance of the Coulomb interaction in the spin-orbit coupling.

It is apparent that the coupling means are very similar for the Racah and SU(3) symmetries, on the other hand they are very different from pure coupling and also much less than for pure L-S coupling. Thus it has been shown that the SU(3) symmetry does not diagonalize the Coulomb interaction and cannot be considered to be a good symmetry approach for the configuration under consideration. This result is similar to that for the $(d+s)^n$ configurations as already noted in the first chapter, where the coupling mean for the $(5d+6s)^2$ configuration of Lu II is larger in SU(3) symmetry than for Racah coupling[4], but in a quantitative study it is

TABLE III

Coupling means of the configuration states (5d+6s)6p of Lu II in different bases.

J	0	1	2	3	4
SU(3) ($\varepsilon\varepsilon'' = 1$)	0.65	0.78	0.69	0.86	1.00
SU(3) ($\varepsilon\varepsilon'' = -1$)	0.90	0.79	0.78	0.86	1.00
Racah	0.99	0.79	0.80	0.86	1.00
L - S	1.00	0.92	0.81	0.90	1.00

TABLE IV

Coupling means of the configurations $(5d+6s)^2p$ of Hf II in different bases

J	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}$	$\frac{9}{2}$	$\frac{11}{2}$
SU(3) ($\varepsilon\varepsilon'' = 1$)	0.48	0.42	0.42	0.45	0.57	0.98
SU(3) ($\varepsilon\varepsilon'' = -1$)	0.47	0.43	0.43	0.44	0.53	0.98
Racah	0.52	0.47	0.45	0.49	0.64	0.98
L - S	0.80	0.68	0.61	0.66	0.65	0.98

shown that for a similar case of La II (which has the same configuration) the value obtained cannot by any means be considered as approaching pure coupling. Thus for the cases considered, even though they appeared favourable, the SU(3) symmetry cannot be considered to be a good approach.

But the role of group theory in the study of the shell model is not restricted to research of symmetry approaches, it also consists of defining bases which are invariant to be used to calculate matrix elements. Thus, while for obvious reasons, the first approach has principally been developed in the theory of nuclear structure, the second, whose value can be judged only by the criteria of simplicity and efficiency, has enabled essential progress to be made in the theory of atomic structure. For example, in atomic spectroscopy, seniority is by no means a good quantum number but nevertheless its introduction has made the analysis of d^n and f^n configurations possible. In the present case the couplings which are proposed seem at first sight to be more complex than Racah coupling, but the chosen bases because of their well-defined symmetry properties possess several advantages and it will be shown in the rest of this chapter how in a relatively simple manner they can be used to great advantage. In this case it is certain that the choice of ε, ε' and ε'' is no longer important and $\varepsilon = \varepsilon' = \varepsilon'' = 1$ has been chosen.

IV. Symmetry of the Operators

a) Single electron operators

The general results of Feneuille[25] lead directly to the fact that the operators $\underset{\sim}{W}^{(K'K)}(\ell_a\ell_b)$ where ℓ_a,ℓ_b belong to the s, d or p electrons can be taken as generators of the group U(18). It is clear furthermore that the infinitesimal operators of a given group U(n) transform as the $(\{2,1^{n-2}\} + \{0\})$ representation of the corresponding group SU(n). Now the group SU(18) allows as a subgroup the direct product SU(2) $\times$ SU(9) with the following reduction

$$\begin{array}{ccc} SU(18) & & SU(2) \times SU(9) \\ \{21^{16}\} + \{0\} & \rightarrow & {}^{1,3}(\{21^{7}\} + \{0\}). \end{array}$$

Also the group SU(9) has the direct product SU(6)(d,s) $\times$ SU(3)(p) as a subgroup and the reduction of a representation of SU(9) of the type $\{2^{\alpha}1^{\beta}\}$ becomes $\{2^{\gamma}1^{\delta}\}\{2^{\theta}1^{\eta}\}$ with the integers γ, δ, θ and η obeying $2\alpha+\beta = 2(\gamma+\theta) + \delta + \eta$, $|\delta-\eta| \leqslant \beta \leqslant \delta+\eta$. This result, the branching rules and the detailed study of the commutation relations leads finally to the classification given in Table V where the operators are defined as

$$\{\{\lambda_1\},\{\lambda_2\},\{\lambda\}\tau\}^{(K'K)}_{\pi q}.$$

b) Two electron operators

The only scalar and symmetric operators which can be constructed from those operators, independent of spin, which have been defined above, have the form:

$$\tfrac{1}{2}[2 - \delta(\mu\mu')\delta(\lambda_1\lambda_1')\delta(\lambda_2\lambda_2')\delta(\lambda\lambda')\delta(\tau\tau')]^{\frac{1}{2}}$$

$$\times \sum_{i>j} (\{\mu\}\{\lambda_1\},\{\lambda_2\},\{\lambda\}\tau\}^{(k)}_i \cdot \{\{\mu'\}\{\lambda_1\},\{\lambda_2'\},\{\lambda'\},\tau'\}^{(k)}_j)$$

$$+ (\{\{\mu'\}\{\lambda_1'\},\{\lambda_2'\},\{\lambda'\}\tau'\}^k_i \cdot \{\{\mu\}\{\lambda_1\},\{\lambda_2\},\{\lambda\}\tau\}^k_j),$$

which can be written more compactly as

$$(\{\{\mu\}\{\lambda_1\},\{\lambda_2\},\{\lambda\}\tau\}^{(k)} \cdot \{\{\mu'\}\{\lambda_1'\},\{\lambda_2'\},\{\lambda\}\tau\}^{(k)})$$

On limitation to Hermitian operators acting within the $(d+s)^m p^n$ configurations 23 operators are obtained and these are listed in Table VI. Starting from these 23 scalar, symmetric Hermitian operators can be constructed which possess the well-defined symmetry of the group SU(3). These are listed in Table VII. It should be noted however that an operator transforming as a $(\sigma_1\sigma_2)$ representation of SU(3) can only be Hermitian when $\sigma_1 = \sigma_2$ since symbolically $(\sigma_1\sigma_2) = (\sigma_2\sigma_1)^\dagger$ and so the Hermitian part of the operator must transform as follows

$$\tfrac{1}{2}[(\sigma_1\sigma_2) + (\sigma_1\sigma_2)^\dagger] = \tfrac{1}{2}[(\sigma_1\sigma_2) + (\sigma_2\sigma_1)].$$

In all of these cases, however, the operators in Table VII are obtained from the single electron operators $(\{\mu\}\{\lambda_1\},\{\lambda_2\};\{\mu'\}\{\lambda_1'\},\{\lambda_2'\}\{\lambda'\};\tau''\{\lambda''\}0)$ which are clearly written as linear combinations of the proceeding operators, i.e. to be specific;

$$\sum_{k\tau\tau'} (\{\lambda\}\tau k + \{\lambda'\}\tau' k|\tau''\{\lambda''\}0)(-1)^k[k]^{-\frac{1}{2}}$$

$$(\{\{\mu\}\{\lambda_1\},\{\lambda_2\},\{\lambda\}\tau\}^{(k)}\{\{\mu'\}\{\lambda_1'\},\{\lambda_2'\}\{\lambda'\}\tau'\}^{(k)})$$

In this expression $\{\lambda''\}$ is a representation of SU(3) which

TABLE V

Single electron operators for the s, p and d electrons

$$\{\{\lambda_1\},\ \{\lambda_2\},\ \{\lambda_3\}\}^{Kk}$$

$\{\lambda_1\}$	$\{\lambda_2\}$	$\{\lambda\}$	operator	designation
(00)	(00)	(00)	$6^{-\frac{1}{2}}[5^{\frac{1}{2}}\underline{W}^{(K0)}(d,d) + \underline{W}^{(K0)}(s,s)]$	$t_1^{(K0)}$
(00)	(00)	(00)	$\underline{W}^{(K0)}(p,p)$	$t_2^{(K0)}$
(00)	(11)	(11)	$\underline{W}^{(K1)}(p,p),\ \underline{W}^{(K2)}(p,p)$	$t_3^{(K1)}, t_3^{(K2)}$
(11)	(00)	(11)	$\underline{W}^{(K1)}(d,d),\ \underline{W}^{(K2)}(\mp +)$	$t_4^{(K1)}, t_4^{(K2)}$
(22)	(00)	(22)	$6^{-\frac{1}{2}}[\underline{W}^{(K0)}(d,d) - 5^{\frac{1}{2}}\underline{W}^{(K0)}(s,s)$	$t_5^{(K0)}$
			$15^{-\frac{1}{2}}[8^{\frac{1}{2}}\underline{W}^{(K2)}(d,d) - 7^{\frac{1}{2}}\overset{+}{\underline{W}}^{(K2)}(d,s)]$	$\overset{+}{t}_5^{(K2)}$
			$\overline{\underline{W}}^{(K2)}(d,s) = 2^{-\frac{1}{2}}[\underline{W}^{(K2)}(d,s) - \underline{W}^{(K2)}(s,d)]$	$\overset{-}{t}_5^{(K2)}$
			$\underline{W}^{(K3)}(d,d),\ \underline{W}^{(K4)}(d,d)$	$t_5^{(K3)}, t_5^{(K4)}$
(20)	(01)	(10)	$6^{-\frac{1}{2}}[5^{\frac{1}{2}}\underline{W}^{(K1)}(d,p) + \underline{W}^{(K1)}(s,p)]$	$t_6^{(K1)}$
		(21)	$6^{-\frac{1}{2}}[5^{\frac{1}{2}}\underline{W}^{(K1)}(s,p) - \underline{W}^{(K1)}(d,p)]$	$t_7^{(K1)}$
			$\underline{W}^{(K2)}(d,p),\ \underline{W}^{(K3)}(d,p)$	$t_7^{(K2)}, t_7^{(K3)}$
(02)	(10)	(01)	$6^{-\frac{1}{2}}[5^{\frac{1}{2}}\underline{W}^{(K1)}(p,d) + \underline{W}^{(K1)}(p,s)]$	$t_8^{(K1)}$
		(12)	$6^{-\frac{1}{2}}[5^{\frac{1}{2}}\underline{W}^{(K1)}(p,s) - \underline{W}^{(K1)}(p,d)]$	$t_9^{(K1)}$
			$\underline{W}^{(K2)}(p,d),\ \underline{W}^{(K3)}(p,d)$	$t_9^{(K2)}, t_9^{(K3)}$

TABLE VI

Spin independent, scalar, symmetric Hermitian two-electron operators within the configurations $(d+s)^n p^m$.

$$(d+s)^n p^m : (t_\alpha^{(k)} . t_\beta^{(k)}) = \tfrac{1}{2}(2 - \delta(\alpha,\beta)) \sum_{i \neq j} . t_{\alpha_i}^{(k)} . t_{\beta_j}^{(k)}$$

Operator	Designation
$(t_1^{(0)} . t_1^{(0)})$	q_1
$(t_2^{(0)} . t_2^{(0)})$	q_2
$(t_1^{(0)} . t_2^{(0)})$	q_3
$(t_3^{(1)} . t_3^{(1)})$	q_4
$(t_3^{(2)} . t_3^{(2)}$	q_5
$(t_4^{(1)} . t_4^{(1)})$	q_6
$(t_4^{(2)} . t_4^{(2)})$	q_7
$(t_3^{(1)} . t_4^{(1)})$	q_8
$(t_3^{(2)} . t_4^{(2)})$	q_9
$(t_5^{(0)} . t_5^{(0)})$	q_{10}
$(t_5^{+(2)} . t_5^{+(2)})$	q_{11}
$(t_5^{-(2)} . t_5^{-(2)})$	q_{12}
$(t_5^{(3)} . t_5^{(3)}$	q_{13}
$(t_5^{(4)} . t_5^{(4)})$	q_{14}
$(t_1^{(0)} . t_5^{(0)})$	q_{15}
$(t_2^{(0)} . t_5^{(0)})$	q_{16}
$(t_3^{(2)} . t_5^{+(2)})$	q_{17}
$(t_4^{(2)} . t_5^{+(2)})$	q_{18}
$(t_6^{(1)} . t_9^{(1)} + (t_7^{(1)} . t_8^{(1)})$	q_{19}

TABLE VI (contd)

Operator	Designation
$(t_6^{(1)} . t_8^{(1)})$	q_{20}
$(t_7^{(1)} . t_9^{(1)})$	q_{21}
$(t_7^{(2)} . t_9^{(2)})$	q_{22}
$(t_7^{(3)} . t_9^{(3)})$	q_{23}

TABLE VII

Spin independent, scalar, symmetric and Hermitian two electron operators within the configurations $(d+s)^n p^m$ with well defined SU_3 symmetry

Symmetry	Operator	Designation
(00)	q_1	Q_1
(00)	q_2	Q_2
(00)	q_3	Q_3
(00)	$\{t_3 \times t_3\}$	Q_4
(00)	$\{t_4 \times t_4\}$	Q_5
(00)	$\{t_3 \times t_4\}$	Q_6
(00)	$\{t_5 \times t_5\}$	Q_7
(00)	q_{20}	Q_8
(00)	$\{t_7 \times t_9\}$	Q_9
(22)	q_{15}	Q_{10}
(22)	q_{16}	Q_{11}
(22)	$\{t_3 \times t_3\}$	Q_{12}
(22)	$\{t_4 \times t_4\}$	Q_{13}
(22)	$\{t_3 \times t_4\}$	Q_{14}
(22)	q_{17}	Q_{15}
(22)	q_{18}	Q_{16}
(22)	$\{t_5 \times t_5\}_a$	Q_{17}
(22)	$\{t_5 \times t_5\}_b$	Q_{18}
(22)	q_{19}	Q_{19}
(22)	$\{t_7 \times t_9\}_a$	Q_{20}
(22)	$\{t_7 \times t_9\}_b$	Q_{21}
(60) + (06)	$\{t_5 \times t_5\}$	Q_{22}
(44)	$\{t_5 \times t_5\}$	Q_{23}

The linear combination $[(60)+(06)]$ is taken to make the operator Hermitian, i.e. $[(60)+(06)]^+ = [(60)^+ + (06)^+]$ $= [(06)+(60)] = [(60)+(06)]$.

simultaneously appears in the reduction of the symmetric product $\{\lambda\}\{\lambda'\}$ and contains the representation D_0 of the group R(3). The symbol τ'' is used to distinguish the similar $\{\lambda''\}$ representations which satisfy these conditions.

The coefficients $(\{\lambda\}\tau k + \{\lambda\}\tau' k|\tau''|\{\lambda''\}0)$ have been calculated by a simple method which relies on the properties of the Casimir operator of the group SU(3). The Casimir operator has the form $\underset{\sim}{V}^{(1)^2} + \underset{\sim}{V}^{(2)^2}$ and the eigenvalues are the same as those in chapter one, namely

$$a(\sigma_1\sigma_2) = \frac{1}{9}(\sigma_1^2 + \sigma_2^2 + \sigma_1\sigma_2 + 3\sigma_1 + 3\sigma_2)(\sigma_1\sigma_2)$$

so it can be shown that:

$$(\{\lambda\}\tau_1 k_1 + \{\lambda'\}\tau_1' k_1|\tau''\{\lambda''\}0) \times [G(\lambda) + G(\lambda') - G(\lambda'')]$$

$$+ 2 \sum_{\tau_2\tau_2' k_2} (\{\lambda\}\tau_2 k_2 + \{\lambda'\}\tau_2' k_2|\tau''\{\lambda''\}0) \times [k_1,k_2]^{-\frac{1}{2}}$$

$$\times \sum_{k=1,2} (\{\lambda\}\tau_1 k_1 \,||\underline{V}^k||\, \{\lambda\}\tau_2 k_2) \times (\{\lambda'\}\tau_1' k_1 \,||\underline{V}^{(k)}||$$

$$\{\lambda'\}\tau_2' k_2)(-1)^k = 0$$

where the reduced matrix elements are defined by

$$[V^k_q, \{\{\mu\}\{\lambda_1\},\{\lambda_2\},\{\lambda\}\tau_2\}^{k_2}_{q_2}] = \sum_{\tau_1 k_1 q_1} (-1)^{k_1-q_1}$$

$$\begin{pmatrix} k & k_2 & k_1 \\ q & q_2 & q_1 \end{pmatrix} (\{\lambda\}\tau_1 k_1 \,||\underline{V}^k||\, \{\lambda\}\tau_2 k_2)$$

$$\times \{\{\mu\}\{\lambda_1\},\{\lambda_2\},\{\lambda\}\tau_1\}^{(k_1)}_{q_1} .$$

Together with the orthonormality relation, this equation is in general sufficient to determine unambiguously the coefficients sought, but it must be pointed out that this is no longer true when the representation $\{\lambda''\}$ appears several times in the symmetric product $\{\lambda\}\{\lambda''\}$, in this case, the ambiguity has been removed in an arbitrary manner as it is usually possible to do. The coefficients $(-1)^k [k]^{-\frac{1}{2}}(\{\lambda\}\tau k + \{\lambda'\}\tau' k \,|\, \tau''\{\lambda''\}0)$ are listed in Table VIII.

Starting with the operators of table VII new operators not only of the group SU_3, but also of the direct product group $SU(3)(d,s)$ $SU(3)(p)$ can be defined and constructed. These operators are defined directly from the following

$$((\{\lambda_1\}\{\lambda_1'\})\{\lambda_1''\},(\{\lambda_2\}\{\lambda_2'\})\{\lambda_2''\},\tau''\{\lambda''\}0)$$

which can themselves be written

$$\sum_{\{\lambda\}\{\lambda'\}}((\{\lambda_1\}\{\lambda_2\})\{\lambda\},(\{\lambda_1'\}\{\lambda_2'\})\{\lambda'\},\{\lambda''\}|(\{\lambda_1\}\lambda\{_1'\})\{\lambda''\},$$
$$(\{\lambda_2\}\{\lambda_2'\})\{\lambda_2''\},\{\lambda''\})\times(\tau\{\lambda_1\}\{\lambda_2\}\{\lambda\},\tau'\{\lambda_1'\}\{\lambda_2'\}\{\lambda'\},\tau''\{\lambda''\}0).$$

The coefficients for the SU_3 group resulting from this development are analogous to the 9-j symbols. They are calculated by the method which depends on the properties of the Casimir operator of the group $SU_3(d,s) \times SU_3(p)$, which is exactly like the Casimir operator quoted previously. All the necessary coefficients are listed in Table IX.

V. Wigner-Eckart Theorem

The operators which have been constructed in the previous paragraph can be considered as a basis on which any scalar symmetric, spin independent Hermitian two particle operators acting within the $(d+s)^n p^m$ configuration can be constructed. This is true in particular for the Coulomb interaction relative to these configurations. The principal

TABLE VIII

Coefficients

$$(-1)^{k}[k]^{-\frac{1}{2}}(\{\lambda\}\tau k + \{\lambda'\}\tau' k|\tau''\{\lambda''\}0)$$

$\{\lambda\} = \{\lambda'\} = (11)$

$\{\lambda''\}$	N-2	k	1	2
(00)	8		1	1
(22)	120		-5	3

$\{\lambda\} = \{\lambda'\} = (22)$

$\{\lambda''\}$	N^{-2}	k	0	2^{+}	2^{-}	3	4
(00)	27		1	1	- 1	1	1
$(22)_a$	480		8	- 4	- 4	-5	3
$(22)_b$	16800		56	20	-28	-5	-29
(06),(60)	9450		56	-25	7	20	- 4
(44)	2520		28	10	14	-5	3

$\{\lambda\} = (21)$, $\{\lambda'\} = (12)$ or $\{\lambda\} = (12)$, $\{\lambda'\} = (21)$

$\{\lambda''\}$	N^{-2}	k	1	2	3
(00)	15		1	1	1
$(22)_a$	210		-7	0	3
$(22)_b$	30		1	-2	1

TABLE IX

Coefficients

$$([(02)(10)\{\lambda\}][(20)(01)\{\lambda'\}]\{\lambda''\}|$$
$$[(02)(20)\{\lambda''_1\}][(10)(01)\{\lambda''_2\}]\{\lambda''\})$$

$\{\lambda''\} = (00)$

$\{\lambda''_1\}$	$\{\lambda''_2\}$	$\{\lambda\}$ / $\{\lambda'\}$	$\begin{Bmatrix}(01)\\(10)\end{Bmatrix}$	$\begin{Bmatrix}(12)\\(21)\end{Bmatrix}$
(00)	(00)		$-(1/6)^{\frac{1}{2}}$	$(5/6)^{\frac{1}{2}}$
(11)	(11)		$(5/6)^{\frac{1}{2}}$	$(1/6)^{\frac{1}{2}}$

$\{\lambda''\} = (22)$

$\{\lambda''_1\}$ $\{\lambda''_2\}$ / $\{\lambda\}$ $\{\lambda'\}$	$\begin{Bmatrix}(01)\\(21)\end{Bmatrix}$	$\begin{Bmatrix}(12)\\(10)\end{Bmatrix}$	$\begin{Bmatrix}(12)\\(21)\end{Bmatrix}_a$	$\begin{Bmatrix}(12)\\(21)\end{Bmatrix}_b$
(22)(00)	$-(1/6)^{\frac{1}{2}}$	$-(1/6)^{\frac{1}{2}}$	$-(7/12)^{\frac{1}{2}}$	$(1/12)^{\frac{1}{2}}$
(11)(11)	$-(1/10)^{\frac{1}{2}}$	$-(1/10)^{\frac{1}{2}}$	$(7/20)^{\frac{1}{2}}$	$(9/20)^{\frac{1}{2}}$
$(22)(11)_a$	$(7/30)^{\frac{1}{2}}$	$(7/30)^{\frac{1}{2}}$	$-(1/15)^{\frac{1}{2}}$	$(7/15)^{\frac{1}{2}}$
$(22)(11)_b$	$(1/2)^{\frac{1}{2}}$	$-(1/2)^{\frac{1}{2}}$	0	0

interest in such a basis lies in the fact that the matrix elements of the operators under consideration between the states of well-defined symmetry in the proposed classification possess very characteristic properties, most of which can be obtained by the Wigner-Eckart theorem. It is clear, for example, that the matrix elements $((d+s)^n S_1\{\lambda_1\}, p^m S_2, \{\lambda\}\tau SL\ M_S\ M_L|Q_\alpha|(d+s)^n S_1'\{\lambda_1'\}, p^m S_2', \{\lambda'\}\tau' SL\ M_S\ M_L)$ of the operators Q_α which transform according to the scalar representation (00) of SU(3) only differ from zero when $\lambda \equiv \lambda'$. Moreover, it can be easily shown that the matrix elements of the operators $Q_1 Q_2 Q_3 Q_4 Q_5$ and Q_7 are diagonal in the proposed scheme, a more detailed examination shows this to be true for the operators Q_6 and $\frac{1}{4}(Q_8 + 15^{\frac{1}{2}} Q_9)$ as well. The eigenvalues obtained for some of the Q_α operators are:

$$Q_1 : \frac{1}{12}\, n(n-1)$$

$$Q_2 : \frac{1}{6}\, m(m-1)$$

$$Q_3 : \frac{1}{18}\, mn$$

$$Q_4 : \frac{1}{48 \times 2^{\frac{1}{2}}}\, [m(14-5m) - 12S_2(S_2+1)]$$

$$Q_5 : \frac{1}{(30) \times 2^{\frac{1}{2}}}\, [9G(\lambda_1) - 10n]$$

$$Q_7 : \frac{1}{180 \times 2^{\frac{1}{2}}}\, [36G(\lambda_1) + 60S_1(S_1+1) + 5n(4n-21)]$$

$$Q_6 : \frac{1}{24 \times (10)^{\frac{1}{2}}}\, [36G(\lambda) - 36G(\lambda_1) - 5m(6-m) + 12S_1(S_1+1)]$$

$$\tfrac{1}{4}(Q_8 + (15)^{\frac{1}{2}} Q_9) : \tfrac{1}{4}[S(S+1) - S_1(S_1+1) - S_2(S_2+1) + \tfrac{1}{2}nm]$$

There is no point in giving further examples but it is worth noting that the treatment adopted for spin independent one and two particle operators can be applied to three particle and spin dependent operators without too much difficulty. These operators will also play an important part in the interpretation of $(d+s)^n p^m$ configurations of the transition elements.

VI. Conclusion

The proposed classification now allows the study of the properties of all of the real and effective interactions within the $(d+s)^n p^m$ configurations in the light of the group SU(3). Even although the SU(3) scheme is no better than the configurational method in the given examples, its symmetry properties make the calculation of the spectroscopic operators and their matrix elements much easier. It would seem that the theory of compact groups has reached the limit of its applicability for the present, and future research in group theory could profitably be directed towards the use of non-compact groups. In the next chapter, a start will be made on the use of non-compact groups in the theory of the harmonic oscillator.

CHAPTER III

MATRIX ELEMENTS OF THE RADIAL-ANGULAR FACTORIZED HARMONIC OSCILLATOR

I. Introduction

The application of non-compact groups to the study of the properties of radial wavefunctions and matrix elements has recently been undertaken by Armstrong[35]. In particular he has shown that it is possible to construct for the hydrogen atom and the isotropic harmonic oscillator radial-like functions of two variables r and t which transform according to the representations of the non-compact group O(2,1) and that in this scheme the positive and negative powers of r have tensorial transformation properties. In the case of the isotropic harmonic oscillator Armstrong[9] has shown that the selection rule

$$\int R_{N'\ell'}\, r^{s+2} R_{N\ell} dr = 0$$

where $|N-N'|$ and s are both even or odd integers and $|N-N'| \geqslant s \geqslant |\ell-\ell'|+1$ holds.

Cunningham[16] following upon Barut[2] has used the scheme $O(4,2) \supset SO(3) \times O(2,1)$ for the hydrogen atom and in this case we shall imbed the group scheme $SO(3) \times O(2,1)$ in the group $Sp(6,R)$. The total wavefunction is factored according to $\psi_{N\ell m}(\theta\varphi r) = Y^m_\ell(\theta\varphi)\, R_{N\ell}(r)$ under the group scheme $Sp(6,R) \supset SO(3) \times O(2,1)$. It is shown that the harmonic oscillator radial functions $R_{N\ell}(r)$ transform according to a single representation of O(2,1) for each ℓ value, and that the quantity $T^k_q = r^{2k}$ for all allowed positive and negative integral and half integral values of k is proportional to the q^{th} component of a tensor operator in O(2,1). The total wavefunction coincides with the normal physical situation and is a function of three variables $\theta\varphi r$.

In the final part of this chapter a comparison is made between this method and that of Armstrong where time enters explicitly. The Wigner-Eckart theorem is shown to hold and the selection rule follows as a consequence. Calculation of the Clebsch-Gordan coefficients allows the matrix elements of r^{2k} to be calculated.

II. The Group Scheme

The 21 generators T_{ij} P_{ij} Q_{ij} with $P_{ij} = P_{ji}$ and $Q_{ij} = Q_{ji}$ $1 \leqslant i,j \leqslant 3$, of Sp(6,R) are defined in terms of their action on the harmonic oscillator wavefunctions written in suitable coordinates. The commutation relations are given by

$$\begin{aligned}
[T_{\alpha\beta}\ T_{\gamma\delta}] &= T_{\alpha\delta}\delta(\gamma\beta) - T_{\gamma\beta}\delta(\alpha\delta) \\
[T_{\alpha\beta}\ P_{\gamma\delta}] &= P_{\alpha\delta}\delta(\gamma\beta) + P_{\alpha\gamma}\delta(\alpha\delta) \\
[T_{\alpha\beta}\ Q_{\gamma\delta}] &= -Q_{\delta\beta}\delta\ (\alpha\gamma) - Q_{\ \gamma\beta}(\alpha\delta) \\
[P_{\alpha\beta}\ Q_{\gamma\delta}] &= -T_{\beta\gamma}\delta(\alpha\delta) - T_{\alpha\gamma}\delta(\delta\beta) - T_{\beta\delta}\delta(\alpha\gamma) - T_{\alpha\delta}\delta(\beta\gamma)
\end{aligned} \qquad \text{(III.1)}$$

where
$$T_{ij} = \tfrac{1}{2}\{a_i^{+}a_j\}$$
$$P_{ij} = \tfrac{1}{2}\{a_i^{+}a_j^{+}\}$$
$$Q_{ij} = \tfrac{1}{2}\{a_i a_j\},$$

with $\{AB\} = AB + BA$, and $a_i = \frac{1}{\sqrt{2}}(r_i+ip_i)$, $a_i^{+} = \frac{1}{\sqrt{2}}(r_i-ip_i)$ as in the normal ladder operator treatment of the harmonic oscillator.

A subgroup SO(3) × O(2,1) can be formed with the SO(3) generators being given by

$$L_+ = (T_{zx} - T_{xz}) + i(T_{zy} - T_{yz})$$

$$L_- = (T_{xz} - T_{zx}) + i(T_{zy} - T_{yz})$$

$$L_0 = i(T_{yx} - T_{xy})$$

with $[L_0 L_\pm] = \pm L_\pm$, $[L_+ L_-] = 2L_0$.

The O(2,1) generators are given by

$$k_0 = \tfrac{1}{2}T_{ii} = \tfrac{1}{2}H, \; H = \text{harmonic oscillator Hamiltonian},$$

$$k_+ = -\tfrac{1}{2}P_{ii}$$

$$k_- = -\tfrac{1}{2}Q_{ii}$$

with $[k_0 k_\pm] = \pm k_\pm$, $[k_+ k_-] = -2k_0$. (III.2)

Consider the whole wavefunction of the harmonic oscillator

$$|N\ell m\rangle = Y_\ell^m(\theta,\varphi)\; R_{N\ell}(r)$$

where $R_{N\ell}(r) = N_{N\ell}(\beta r^2)^{\ell/2}\; e^{-r^2/2}\; L^{\ell+\frac{1}{2}}_{\frac{1}{2}(N-\ell)}\;(\beta r^2)$ (III.3)

and $N_{N\ell} = \left[\dfrac{\beta^3[\frac{1}{2}(N-\ell)]!}{2[\frac{1}{2}(N+\ell+1)]!}\right]^{\frac{1}{2}}$

with the implication that $(X)! = \Gamma(X+1)$. In order to simplify the system the following set of units is used. $\hbar = m = w = 1$ which gives $\beta = 1$ and now put $\beta r^2 = z$ so that the radial wave equation becomes

$$R_{N\ell}(z) = N_{N\ell}\; z^{\ell/2}\; e^{-z/2}\; L^{\ell+\frac{1}{2}}_{\frac{1}{2}(N-\ell)}(z),$$

with a Hilbert space being defined by the inner product

$$\int_0^\infty \int_\Omega R_{N'\ell'}(z) Y_{\ell'}^m(\theta,\varphi) z^{\frac{1}{2}} R_{N\ell} Y_\ell^m(\theta,\varphi) d\Omega \, \frac{dz}{2} = \delta(NN')\delta(\ell\ell') \quad (III.4)$$

where $d\Omega = \sin\theta d\theta d\varphi$. In the scheme $Sp(6,R) \supset SO(3) \times O(2,1)$ the wavefunctions of fixed m form a basis of a representation of O(2,1) since

$$\begin{aligned} k_+|N\ell> &= \tfrac{1}{2}[(N+\ell+3)(N-\ell+2)]^{\frac{1}{2}}|N+2\ell> \\ k_-|N\ell> &= \tfrac{1}{2}[(N-\ell)(N+\ell+1)]^{\frac{1}{2}}|N-2\ell> \\ k_0|N\ell> &= \tfrac{1}{2}(N+\tfrac{3}{2})|N\ell> \end{aligned} \quad (III.5)$$

where $|N\ell> = R_{N\ell}(z)$, where N runs from ℓ upwards and $N-\ell$ is an even integer.

It should now be noted that there is no upper bound to the positive (O(2)) quantum number N and that the lower bound of the representation is given by $N = \ell$, this representation can be shown to be unitary and irreducible.

A realization of the operators in Hilbert space is

$$\begin{aligned} k_\pm &= \pm(z\frac{d}{dz} \mp \frac{z}{2} \pm \frac{H}{2} + \frac{3}{4}) \\ k_0 &= \tfrac{1}{2}H \end{aligned} \quad (III.6)$$

where H is the Hamiltonian of the 3-dimensional isotropic harmonic oscillator. Observation of the equations 5 and 6 leads directly to the conclusion that the substitutions $a = \frac{1}{2}(\ell-\frac{1}{2})$ and $b = \frac{1}{2}(N+\frac{3}{2})$ will simplify the equations to give

$$\begin{aligned} k_\pm|ab> &= [(b\mp a)(b\pm a\pm 1)]^{\frac{1}{2}}|ab\pm 1> \\ k_0|ab> &= b|ab> \end{aligned} \quad (III.7)$$

where $|N\ell\rangle \rightarrow |ab\rangle$ and $|N-1\ \ell+1\rangle \rightarrow |a+\frac{1}{2}, b-\frac{1}{2}\rangle$ and equation 3 becomes

$$|ab\rangle = \left[\frac{(b-a-1)!}{2(a+b)!}\right]^{\frac{1}{2}} z^{a+\frac{1}{4}}\, e^{-z/2}\, L^{2a+1}_{b-a-1}(z) \qquad \text{(III.8)}$$

with $b \geqslant a+1$ and a and b may be integral or half integral with the proviso that $(b-a-1)$ be integral.

Formation of the Casimir operator

$$G = k_0{}^2 - \tfrac{1}{2}(k_+k_- + k_-k_+)$$

so that $G|ab\rangle = a(a+1)|ab\rangle$

$$\text{i.e. } G|N\ell\rangle = \tfrac{1}{4}\{\ell(\ell+1) - \tfrac{3}{4}\} \qquad \text{(III.9)}$$

Barut and Fronsdal[39] have shown that the eigenvalues of the Casimir operator G are given by

$$G|\varphi m\rangle = \varphi(\varphi+1)|\varphi m\rangle.$$

If a representation is bounded below, its lower bound is $-\varphi$ and if φ is negative the representation is unitary and labelled $D^+_{-\varphi}$. This implies that the wavefunctions $|ab\rangle$ for a fixed m form a basis for the unitary irreducible representation $D^+_{a+1} = D^+_{\frac{1}{2}(\ell+\frac{3}{2})}$. It should be noted here that the realization of O(2,1) is a projective one.

III. Tensorial Properties of z^k

The quantity $T^k_q = z^k$ where k may be positive or negative integral or half integral, transforms as the q^{th} component of an O(2,1) tensor operator with the associated representation depending on the size of k relative to zero.

Following Infeld and Hull[36] we define

$$A^{\ell}_{\ell+1} = \left[\frac{(2\ell+3)}{(\ell+1-m)(\ell+1+m)(2\ell+1)}\right]^{\frac{1}{2}} \{(\ell+\tfrac{1}{2})\cos\theta + \sin\theta\frac{d}{d\theta}\}$$
(III.10)

Replacing ℓ by a gives

$$A^{2a}_{2(a+\frac{1}{2})} = \left[\frac{(4a+3)}{(2a+1-m)(2a+1+m)(4a+1)}\right]^{\frac{1}{2}} \{(2a+\tfrac{1}{2})\cos\theta + \sin\theta\frac{d}{d\theta}\}$$
(III.11)

so that $A^{2a'}_{2a}$ can be built up as products of $A^{2a}_{2(a+\frac{1}{2})}$ and $A^{2a}_{2(a-\frac{1}{2})}$.

From the relation

$$\langle a'\ b+q\pm1|[k_{\pm}T^{k}_{q}]A^{2a'}_{2a}|ab\rangle$$

$$= \pm\langle a'\ b+q\pm1|\Big\{\{z\frac{d}{dz} \mp \frac{z}{2} \pm (b+q) + \tfrac{3}{4}\}z^{k}$$

$$- z^{k}\{z\frac{d}{dz} \mp \frac{z}{2} \pm b + \tfrac{3}{4}\}\Big\}A^{2a'}_{2a}|ab\rangle$$

$$= (q\pm k)\langle a'\ b+q\pm1|A^{2a'}_{2a}\ T^{k}_{q\pm1}|ab\rangle$$

we obtain

$$[k_{\pm}\ T^{k}_{q}] = (q\pm k)T^{k}_{q\pm1} \qquad \text{(III.12)}$$

If $k < 0$ the representation is at finite dimension $(-2k+1)$ and is labelled D_{-k} and is non-unitary, hence the tensor operator can be normalized in an arbitrary manner. If $k \geqslant 0$ the representation is infinite dimensional and reducible, but not fully reducible for while the spaces $q \leqslant -k$ and $q \geqslant k$ are invariant under the group operations the space $-k+1 \leqslant q \leqslant k-1$ is not. This type of representation is called indecomposible and has been studied by Barut and Phillips[37]. These representations are labelled as D'_{k-1} and are non-unitary since the eigenvalues of $k_{\pm}k_{\mp}$ are not positive definite. Again the tensor operator may be normalized in an arbitrary manner, and this will be done in a later section.

IV. The Wigner-Eckart Theorem

The most common way of proving the Wigner-Eckart Theorem for the group SO(3) is to set up recursion relations between different matrix elements of the q^{th} and $(q+1)^{th}$ components of an SO(3) tensor operator and to show that these are identical to the recursion relations for the corresponding SO(3) Clebsch-Gordan coefficients. This implies that the matrix elements and the Clebsch-Gordan coefficients are proportional, the proportionality constant being the reduced matrix element.

The proof requires that if $J_i|\ell m\rangle = a_i|\ell m_i\rangle$ then $[J_i T^{\ell}_{m}] = a_i T^{\ell}_{m_i}$ where J_i is a SO(3) generator, $T^{\ell}_{m_i}$ is a SO(3) tensor operator, and that the states being coupled be orthonormal.

In the O(2,1) case the states corresponding to D_{-k} and D'_{k-1} are written as $|kq\rangle$ where k and q serve to distinguish them from the states $|ab\rangle$ of D^{+}_{a+1}. The corresponding tensor operator is written as $N_{kq} z^{k} A^{2a'}_{2a}$ where N_{kq} is a normalization factor, thus

$$k_{\pm}|kq\rangle = (q\pm k)\,\frac{N_{kq}}{N_{kq\pm 1}}\,|k\;q\pm 1\rangle \tag{III.13}$$

and

$$[k_{\pm}\;T^{k}_{q}] = (q\pm k)\,\frac{N_{kq}}{N_{kq\pm 1}}\,T^{k}_{q\pm 1} \tag{III.14}$$

Furthermore,

$$k_{0}|kq\rangle = q|kq\rangle \tag{III.15}$$

$$[k_{0}\;T^{k}_{q}] = q\,T^{k}_{q}. \tag{III.16}$$

As the states $|ab\rangle$ are orthonormal the Wigner-Eckart theorem is valid and the following expression can be written

$$\langle abm|T^k_q|a'b'm\rangle = C^{a\ k\ a'}_{b\ q\ b'} \langle a\,||\underline{T}^k||\,a'\rangle. \tag{III.17}$$

where $C^{a\ k\ a'}_{b\ q\ b'}$ is an O(2,1) Clebsch-Gordan coefficient, coupling the states $D^+_{a'+1}$ with either the states of D'_{-k} or D'_{k-1}, normalized as above, to yield the states of D^+_{a+1} and $\langle a\,||T^k||\,a'\rangle$ is the reduced matrix element dependent only on a, a' and k.

V. <u>The Racah Algebra and Calculation of the Clebsch-Gordan Coefficients</u>

Following the method of Cunningham[16], which was derived from the methods of Van der Waerden[38] and Bargmann[15], the process of coupling two representations and the contragradient of a third to form an invariant is used.

To use this technique the representations must be realized in terms of multispinors $N_{ab}\xi^a\eta^b$ where N_{ab} is a normalization constant for the representations of O(2,1) or SO(3). In this realization

$$k_0 = \tfrac{1}{2}\left(\xi\frac{\partial}{\partial\xi} - \eta\frac{\partial}{\partial\eta}\right) \tag{III.18}$$

$$k_+ = \xi\frac{\partial}{\partial\eta}, \qquad k_- = \eta\frac{\partial}{\partial\xi} \tag{III.19}$$

so that $k_0\ N_{ab}\xi^a\eta^b = \tfrac{1}{2}(a-b)\ N_{ab}\xi^a\eta^b$

and $$G\ N_{ab}\xi^a\eta^b = \tfrac{1}{4}(a-b)(a-b+2)\ N_{ab}\xi^a\eta^b. \tag{III.20}$$

Hence, if the eigenvalues of a and k_0 are $\varphi(\varphi+1)$ and m respectively, then the states are represented by $N_{ab}\xi^{\varphi+m}\eta^{\varphi-m}$ where N_{ab} has been shown by Barut and Fronsdal[39] to be

$$\left[\frac{(m-1-\varphi)!}{(m+\varphi)!}\right]^{\frac{1}{2}}$$

for the unitary representations $D^{+}\varphi$. But note here that N_{ab} is arbitrary for non-unitary representations.

The contragredient of a quantity is defined as follows. Consider the state

$$|\varphi m\rangle = \frac{(\xi\ )^{\varphi+m}(\eta)^{\varphi-m}}{[(\varphi+m)!(\varphi-m)!]^{\frac{1}{2}}} \tag{III.21}$$

where ξ and η are fermion or boson operators, then the contragredient is defined such that

$$\sum_{mm'} |\varphi m\rangle|\varphi m'\rangle = F(\varphi)|\varphi 0\rangle$$

where $F(\varphi)$ is a function of φ alone and the state $|\varphi 0\rangle$ represents a state which is invariant under the group operations. Now as $m+m' = M$ and $M = 0$, i.e. a function invariant under group operations. We get

$$\sum_{m} |\varphi m\rangle|\varphi -m\rangle(-1)^{\varphi-m} = F(\varphi)|\varphi 0\rangle \tag{III.22}$$

where $F(\varphi)|\varphi 0\rangle$ is a state with zero 'angular momentum' and is invariant under group operations, so $|\varphi -m\rangle(-1)^{\varphi-m}$ is said to be the contragredient of $|\varphi m\rangle$. Now if the states are written as

$$|\varphi m\rangle = N_m \xi^{\varphi-m}\eta^{\varphi+m}$$

then the contragredient is $N_m \xi^{\varphi-m}\eta^{\varphi+m}(-1)^{\varphi-m}$. Consider the Kronecker product $D_1 \otimes D_2 \subset D_3$ where D_1, D_2 and D_3 are representations of the group under consideration. The Clebsch-Gordan coefficient is by definition that function which reduces the Kronecker product $D_1 \otimes D_2$ to D_3. If we form the contragredient representation $\hat{D}_3$ then from equation III.22 $D_3 \otimes \hat{D}_3$ must be invariant under the group operations.

Hence the triple product $D_1 \otimes D_2 \otimes \hat{D}_3$ contains an invariant I under the group operations thus we may write

$$I = \sum_{m_1 m_2 m_3} F(\varphi_1\varphi_2\varphi_3)\, C^{\varphi_1\varphi_2\varphi_3}_{m_1 m_2 m_3}\, N_1 N_2 N_3\, \xi_1^{\varphi_1+m_1}\, \eta_1^{\varphi_1-m_1}$$

$$\xi_2^{\varphi_2+m_2}\, \eta_2^{\varphi_2-m_2}\, \xi_3^{\varphi_3-m_3}\, \eta_3^{\varphi_3+m_3}\, (-1)^{\varphi_3-m_3} \qquad \text{(III.24)}$$

where I is an invariant in the space of polynomials $\prod_i \xi_i^{a_i}\eta_i^{b_i}$. However, since the representation matrices are unimodular the only invariants in this space are the three determinants

$$\delta_1 = \xi_2\eta_3 - \xi_3\eta_2, \quad \delta_2 = \xi_3\eta_1 - \xi_1\eta_3, \quad \delta_3 = \xi_1\eta_2 - \xi_2\eta_1$$

and every monomial in these. Hence

$$\delta_1^{k_1}\delta_2^{k_2}\delta_3^{k_3} = (\xi_2\eta_3 - \xi_3\eta_2)^{k_1}(\xi_3\eta_1 - \xi_1\eta_3)^{k_2}(\xi_1\eta_2 - \xi_2\eta_1)^{k_3} \qquad \text{(III.25)}$$

$$= \sum_{pqr} (-1)^{p+q+r}\binom{k_1}{p}\binom{k_2}{q}\binom{k_3}{r}\xi_1^{k_3+q-r}\,\xi_2^{k_1+r-p}\,\xi_3^{k_2+p-q}\,\eta_1^{k_2+r-q}$$

$$\eta_2^{k_3+p-r}\,\eta_3^{k_1+q-p} \qquad \text{(III.26)}$$

Equating coefficients of III.24 and III.26 leads directly to

$$\begin{aligned} k_3+q-r &= \varphi_1+m_1 \\ k_2+r-q &= \varphi_1-m_1 \\ k_1+r-p &= \varphi_2+m_2 \\ k_3+p-r &= \varphi_2-m_2 \\ k_2+p-q &= \varphi_3-m_3 \\ k_1+q-p &= \varphi_3+m_3 \end{aligned}$$

so that

$$k_2+k_3 = 2\varphi_1, \qquad k_1+k_3 = 2\varphi_2, \qquad k_1+k_2 = 2\varphi_3$$

also

$$q-r = \varphi_3-\varphi_2+m_1$$
$$r-p = \varphi_1-\varphi_3+m_2$$
$$p-q = \varphi_2-\varphi_1-m_3$$

which leads to the selection rule $m_1+m_2 = m_3$. Equating coefficients of III.24 and III.26 also leads to

$$F(\varphi_1\varphi_2\varphi_3)N_1N_2N_3\ C^{\varphi_1\varphi_2\varphi_3}_{m_1m_2m_3}\ (-1)^{\varphi_3-m_3}$$
$$= \sum_{pqr}\ (-1)^{p+q+r}\binom{k_1}{p}\binom{k_2}{q}\binom{k_3}{r} \qquad \text{(III.27)}$$

We may eliminate p and q by use of

$$p = \varphi_3-\varphi_1-m_2+r$$

and

$$q = \varphi_3-\varphi_2+m_1+r$$

which gives

$$p+q+r = 2\varphi_3-\varphi_1-\varphi_2+m_1-m_2+3r \qquad \text{(III.28)}$$

Finally

$$F(\varphi_1\varphi_2\varphi_3)N_1N_2N_3\ C^{\varphi_1\varphi_2\varphi_3}_{m_1m_2m_3}(-1)^{\varphi_3-m_3}$$
$$= \sum_{r}\ (-1)^{2\varphi_3-\varphi_1-\varphi_2+m_1-m_2+3r}\binom{k_1}{\varphi_3-\varphi_1-m_2+r}\binom{k_2}{\varphi_3-\varphi_2+m_1+r}\binom{k_3}{r}$$
$$\text{(III.29)}$$

It is instructive at this point to derive the Clebsch-Gordan coefficients for SO(3), as equation III.29 is a general form suitable for use in both the O(2,1) and the SO(3) groups. For SO(3) all of k_1, k_2 and k_3 must be positive, so substitution of $\varphi_1 = \ell_1$, $\varphi_2 = \ell_2$ and $\varphi_3 = \ell_3$ gives

$$F(\ell_1\ell_2\ell_3)N_1N_2N_3\, C^{\ell_1\ell_2\ell_3}_{m_1m_2m_3}\,(-1)^{\ell_3-m_3} = \sum_r (-1)^{2\ell_3-\ell_1-\ell_2+m_1-m_2+3r}$$

$$\times \frac{(\ell_1+\ell_2-\ell_3)!(\ell_1-\ell_2+\ell_3)!(-\ell_1+\ell_2+\ell_3)!}{r!(\ell_2+m_2-r)!(\ell_3-\ell_1-m_2+r)!(\ell_3-\ell_7+m_1+r)!(\ell_1-m_1-r)!(\ell_1+\ell_2-\ell_3-r)!}$$

(III.30)

Substituting for N_1, N_2 and N_3 we get

$$F(\ell_1\ell_2\ell_3)\, C^{\ell_1\ell_2\ell_3}_{m_1m_2m_3} = [(\ell_1+m_1)!(\ell_2+m_2)!(\ell_3+m_3)!(\ell_1-m_1)!(\ell_2-m_2)!$$

$$\times (\ell_3-m_3)!]^{\frac{1}{2}}(\ell_1+\ell_2-\ell_3)!(\ell_1-\ell_2+\ell_3)!(-\ell_1+\ell_2+\ell_3)!$$

$$\times \sum_r \frac{(-1)^{-\ell_1-\ell_2+\ell_3+r-2m_1}}{r!(\ell_1-m_1-r)!(\ell_2+m_2-r)!(\ell_3-\ell_1-m_2+r)!(\ell_3-\ell_2+m_1+r)!(\ell_1+\ell_2-\ell_3-r)!}$$

(III.31)

The orthonormality condition puts the following condition on the coefficients.

$$\sum_{m_1} C^{\ell_1\ell_2\ell_3}_{m_1m_2m_3}\, C^{\ell_1\ell_2\ell_3}_{m_1m_2m_3} = 1 \qquad \text{(III.32)}$$

Selecting $m_3 = \ell_3$ so that $m_1+m_2 = \ell_3$ we get the requirement that $\ell_1-m_1 = r$ in the summation so that

$$\sum_{m_1} (-1)^{2(\ell_3-\ell_1-\ell_2-2m_1+r)}\, F^{-2}(\ell_1\ell_2\ell_3)\, \frac{(\ell_1+m_1)!(\ell_2+\ell_3-m_1)!}{(\ell_2-\ell_3+m_1)!(\ell_1-m_1)!}$$

$$\times (2\ell_3)!(\ell_1+\ell_2-\ell_3)!^2 = 1$$

i.e.

$$\sum_{m_1} (-1)^{2(\ell_3-\ell_2-\ell_1)}\, F^{-2}(\ell_1\ell_2\ell_3)\, \frac{(\ell_1+m_1)!(\ell_2+\ell_3-m_1)!(2\ell_3)!}{(\ell_2-\ell_3+m_1)!(\ell_1-m_1)!}$$

$$\times (\ell_1+\ell_2-\ell_3)!^2$$

Now sum out the m_1 dependence (Edmonds[40] page 121, A13) to get

$$F(\ell_1\ell_2\ell_3) = (-1)^{(\ell_3-\ell_2-\ell_1)} \left[\frac{(\ell_1+\ell_2+\ell_3+1)!(\ell_1+\ell_2-\ell_3)!(\ell_1-\ell_2+\ell_3)!(-\ell_1+\ell_2+\ell_3)!}{(2\ell_3+1)}\right]^{\frac{1}{2}}$$

Hence at last the SO(3) Clebsch-Gordan coefficient is found to be,

$$C^{\ell_1\ell_2\ell_3}_{m_1m_2m_3} = \delta(m_3,m_1+m_2)\left[\frac{(2\ell_2+1)(\ell_1+\ell_2-\ell_3)!(\ell_1-\ell_2+\ell_3)!(-\ell_1+\ell_2+\ell_3)!}{(\ell_1+\ell_2+\ell_3+1)!}\right]^{\frac{1}{2}}$$

$$\times\ [(\ell_1-m_1)!(\ell_2-m_2)!(\ell_3-m_3)!(\ell_1+m_1)!(\ell_2+m_2)!(\ell_3+m_3)!]^{\frac{1}{2}}$$

$$\times \sum_r \frac{(-1)^r}{r!(\ell_1+\ell_2-\ell_3-r)!(\ell_1-m_1-r)!(\ell_1+m_2+r)!(\ell_3-\ell_2+m_2+r)!(\ell_3-\ell_1-m_2+r)!} \qquad \text{(III.34)}$$

as is already well known.

<u>Derivation of some of the O(2,1) Clebsch-Gordan coefficients</u>

Coefficients reducing the product $D^+(\varphi_1) \otimes D^+(\varphi_2)$ to $D^+(\varphi_3)$, i.e. coupling two positive discrete series to give a positive discrete series can be derived from equation III.29. Noting that the positive discrete representations are labelled by $\varphi = -a-1$ which comes from a solution of the Casimir equation $\varphi(\varphi+1) = a(a+1)$, we get

$$F(a_1a_2a_3)N_1N_2N_3\, C^{a_1a_2a_3}_{b_1b_2b_3}\, (-a)^{-a_3-1-b_3} \sum_r (-1)^{2a_3-a_1-a_2+b_1-b_2+3r}$$

$$\binom{k_1}{a_3-a_1-b_2+r}\binom{k_2}{a_3-a_2+b_1+r}\binom{k_3}{r} \qquad \text{(III.35)}$$

with $k_1 = a_1-a_2-a_3-1$, $k_2 = -a_1+a_2-a_3-1$, $k_3 = -a_1+a_2+a_3-1$. Now these may be normalized using the orthonormality properties of the O(2,1) Clebsch-Gordan coefficients, namely that

$$\sum_{b_1 b_2} C^{a_1 a_2 a_3}_{b_1 b_2 b_3} \, C^{*\,a_1 a_2 a_2}_{\;\;b_1 b_2 b_3} = 1$$

and this finally leads to the Clebsch-Gordan coefficient.

$$C^{a_1 a_2 a_3}_{b_1 b_2 b_3} = (-2a_3-1)^{\frac{1}{2}}$$

$$\left[\frac{(-a_1-a_2-a_3-2)!(a_1+a_2-a_3)!(b_3+a_3)!(b_1+a_1)!(b_2+a_2)!}{(a_2-a_1-a_3-1)!(a_1-a_2-a_3-1)!(b_1-a_1-1)!(b_2-a_2-1)!(b_3-a_3-1)!}\right]^{\frac{1}{2}}$$

$$\sum_r \frac{(-1)^r \quad (b_2+a_1-a_3-1-r)!(b_1-a_1-1+r)!}{r!(b_1+a_3-a_2+r)!(b_2+a_2-r)!(a_1+a_2-a_3-r)!} \qquad \text{(III.36)}$$

which agrees with the formula derived by Holman and Biedenharn[50]. By a similar method the coefficients coupling $D^-(\varphi_1) \times D^-(\varphi_2)$ to $D^-(\varphi_3)$ can be calculated; the Clebsch-Gordan coefficient so derived is similar to that of III.36 except that $b_i \rightarrow -b_i$ $i = 1,2,3$.

The case in which we are most interested is the one where an infinite discrete representation is coupled to a finite or undecomposible representation to an infinite discrete representation. Firstly we will couple the positive discrete representation $D^+(\varphi_1)$ to the finite representation $D'(k-1)$ to give the positive discrete representation $D^+(\varphi_3)$. In order that the correct representations be coupled k_1 and k_3 must be positive and k_2 negative which are satisfied by the required substitutions $\varphi_1 = -a-1$, $\varphi_2 = -k$ and $\varphi_3 = -a'-1$. Where we note that $k < 0$ then on substitution into eq. III.29 we find

$$F(aka')N_1N_2N_3 \, C^{a\ k\ a'}_{b\ q\ b'} \, (-1)^{-a'-1-b} = \sum_r (-1)^{-2a'-2+k+a+1+b-q+3r}$$

$$\times \binom{-a'-k+a}{-a'+a-q+r}\binom{-a'-a+k-2}{-a'+b+k-1+r}\binom{-a+a'-k}{r} \qquad k < 0 \qquad \text{(III.37)}$$

which may be written

$$C^{a\,k\,a'}_{b\,q\,b'} = (N_1N_2N_3)^{-1}F(a\,k\,a')^{-1} \sum_r (-1)^{b+b'+k-q-a'+r}$$

$$\binom{a-k-a'}{a-a'-a+r}\binom{k-a-a'-2}{k+b-a'-1+r}\binom{a'-a-k}{r} \qquad k < 0 \qquad \text{(III.38)}$$

Now as we are dealing with non-unitary representations the Clebsch-Gordan coefficients cannot be normalized without some assumptions being made, generally the normalization is chosen so that the Clebsch-Gordan coefficients derived are very similar to the SO(3) Clebsch-Gordan coefficients. We shall derive the normalization as a consequence of the properties of the tensor operator $T^k_q = r^{2k}$ of the harmonic oscillator in the group O(2,1).

Consider the product state $|kq;ab\rangle$ where $|kq\rangle$ corresponds to the tensor operator T^k_q and the states $|ab\rangle$ form a basis of the representation $D^+(a+1)$, so that in this basis $k^+_\pm = k_\mp$ under the inner product $\langle a'b'|ab\rangle = \delta(aa')\delta(bb')$. Now the set $|kq\rangle$ does not form the basis of a unitary representation so that $k^+_\pm = k_\mp$ in the direct product space can be met only if the inner product is defined as

$$\langle k'q'|kq\rangle = (-1)^q\delta(q'q),$$

this is the case since

$$\langle k'q'|k_\pm\,k\,q\rangle = \mp[(k\mp q)(k\pm q\pm 1)]^{\frac{1}{2}}\langle k'q'|kq\rangle$$

$$\therefore \quad \langle k'q'|k_\pm\,k\,q\rangle = \mp\,(-1)^q[(k\mp q)(k\pm q\pm 1)]^{\frac{1}{2}}$$

$$= \langle k_\pm\,k'\,q'|kq\rangle$$

Thus if $|ab\rangle = \sum_{b'q} C^{a'\,k\,a}_{b'\,q\,b}|a'b';kq\rangle$ with N_2 chosen as

$[(k-q)!(k+q)!]^{-\frac{1}{2}}$. Taking the inner product with $\langle kq;a''b''|$ leads directly to the orthogonality condition

$$\sum_{bq} C^{a\,k\,a'}_{b\,q\,b'}\; C^{*a\,k\,a''}_{\;\;b\,q\,b''}\,(-1)^q = \delta(a'a'')\delta(b'b'') \qquad \text{(III.39)}$$

Now for the case of $k \geqslant 0$ in this $\varphi_2 \geqslant 0$ so that both of k_1 and k_3 cannot be negative and on taking $a \geqslant a'$ the following substitutions $\varphi_1 = -a-1$, $\varphi_3 = -a'-1$ and $\varphi_2 = k$ lead to the result,

$$F(a\,k\,a')\,N_1N_2N_3\,C^{a\,k\,a'}_{b\,q\,b'} = \Sigma(-1)^{-a'-k+a+b+b'-q+r}$$

$$\times\binom{a+k-a'}{a-a'-q+r}\binom{-a'-a-k-2}{-k+b-a'-a+r}\binom{a'+k-a}{r} \qquad k \geqslant 0 \qquad \text{(III.40)}$$

Putting $a \geqslant a'$ two possible cases arise, either both of $a-a'+k$ and $a'-a+k$ are positive or $a-a'+k$ positive and $a'-a+k$ negative. By choosing $N_2 = [(k-q)!(k+q)!]^{-\frac{1}{2}}$ and similarly for N_1 and N_3 the Clebsch-Gordan coefficient becomes after normalization

$$C^{a\,k\,a'}_{b\,q\,b'} = [(k+q)!(k-q)!(b-a)!(b+a)!(b'+a')!(b'-a')!]^{\frac{1}{2}}$$

$$\times\,(-2a'+1)^{\frac{1}{2}}\left[\frac{(-a+k+a')!(a-k+a')!(a+k-a')!}{(a+a'+k+1)!}\right]^{\frac{1}{2}}$$

$$\times\sum_r \frac{(-1)^r\,(b+a+r)!}{r!(a'+k-a-r)!(a-a'-q+r)!(k+q-r)!(b-k-a'-1+r)!} \qquad \text{(III.41)}$$

Now after some rearrangement this Clebsch-Gordan coefficient can be related to a standard SO(3) Clebsch-Gordan coefficient by

$$C^{a\,k\,a'}_{b\,q\,b'} = C(aba'b'\,|\,aa'kq)$$

where

$C = -1$: $a-a'$ odd

$C = -1$: $a-a'$ $\frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \ldots$

$C = 1$: $a-a'$ even

$C = i$: $a-a'$ $\frac{1}{2}, \frac{5}{2}, \frac{9}{2}, \ldots$

A similar relationship is found for the Clebsch-Gordan coefficients for $k < 0$. The selection rule on the operator T^k_q imposed by the O(2,1) Clebsch-Gordan coefficients is $|N-N'| > 2k > |\ell-\ell'|$ for $k \geqslant 0$ and $|N-N'| < -2k < |\ell-\ell'|$ for $k < 0$, when both of $|N-N'|$ and $2k$ are even or odd integers lead to zero matrix elements.

VI. Reduced Matrix Elements

The reduced matrix elements of a tensor operator T^k_q can be calculated using the relation

$$\langle a'a|T^k_0|aa\rangle = C^{a\ k\ a'}_{a\ 0\ a} \langle a'||\underline{T}^k||a\rangle$$

where $a \geqslant a'$ and the left-hand side is equivalent to

$$\int_\Omega \int_\infty R_{\ell\ell} r^{2k} R_{\ell'\ell} r^2 dr d\Omega$$

which evaluates to

$$\frac{(2k+\ell+\ell'+1)!!}{[2^{2k}(2\ell+1)!!(2\ell'+1)!!]^{\frac{1}{2}}} \qquad \text{(III.42)}$$

The very specialised Clebsch-Gordan coefficient $C^{a\ k\ a'}_{a\ 0\ a}$ evaluates to

$$(2k+2a+2a'+2)!! \times \left[\frac{(a+a'-k)!}{2^{2k}(4a+2)!!(4a'+2)!!(a+a'+k+1)!(a-a'+k)!(a'-a+k)!}\right]^{\frac{1}{2}}$$

and so the reduced matrix element becomes

$$\langle a \,\|\underline{T}^k\|\, a'\rangle = \left[\frac{(a+a'+k+1)!\,(a-a'+k)!\,(a'-a+k)!}{(a+a'-k)!}\right]^{\frac{1}{2}} \qquad k \geqslant 0$$

(III.44)

Matrix elements of T^k_q $k \geqslant 0$ can be readily calculated, e.g.

$$\langle N\ell|r|N+1 \;\; \ell+1\rangle \equiv \langle ab|T^{\frac{1}{2}}_{-\frac{1}{2}}|a+\tfrac{1}{2},\; b-\tfrac{1}{2}\rangle$$

$$= \frac{(-1)^{a+b}}{0!\,(1)!}\,(a\; b\; a+\tfrac{1}{2}\;\; b+\tfrac{1}{2}|\tfrac{1}{2}\;\; -\tfrac{1}{2})\langle a\,\|T^{\frac{1}{2}}\|\,a'\rangle$$

$$= i(-1)^{a+b}\begin{pmatrix} a & \frac{1}{2} & a+\frac{1}{2} \\ b & \frac{1}{2} & -(b+\frac{1}{2}) \end{pmatrix}(-1)^{2a+1}\langle a\,\|T^{\frac{1}{2}}\|\,a'\rangle$$

$$= -(a+b+1)^{\frac{1}{2}}$$

$$= -\left(\frac{N+\ell+3}{2}\right)^{\frac{1}{2}} . \qquad \text{(III.45)}$$

Hence $\quad \langle N\ell|r|N+1 \;\; \ell+1\rangle = -\left(\frac{N+\ell+3}{2}\right)^{\frac{1}{2}}$

Similarly

$$\langle N\ell|r^3|N+3 \;\; \ell+1\rangle \equiv \langle ab|T^{3/2}_{-3/2}|a+\tfrac{1}{2}\;\; b+\tfrac{3}{2}\rangle$$

$$= [(a+b+1)(a+b+2)(b-a)]^{\frac{1}{2}}$$

$$= \left\{\left(\frac{N+\ell+3}{2}\right)\left(\frac{N+\ell+5}{2}\right)\left(\frac{N-\ell+2}{2}\right)\right\}^{\frac{1}{2}} \qquad \text{(III.46)}$$

A table of matrix elements for r^{2k} $k \geqslant 0$ is given by Shaffer[41] for N' and ℓ' up to $N \pm 4$ and $\ell \pm 4$ respectively. The case for $k < 0$ requires some attention; the Clebsch-Gordan coefficients for $k < 0$ can be calculated in a similar manner to that used to calculate them for $k \geqslant 0$. On completing the derivation a relationship is formed as follows.

$|k| > |q|, \quad k < 0$

$$\langle ab|T^k_q|a'b'\rangle = \frac{(-1)^{k+q}}{(-k-q)!\,(-k+q)!}\begin{pmatrix} a' & -(1+k) & a \\ -b' & q & b \end{pmatrix}\langle a\,\|T^k\|\,a'\rangle$$

where

$$\langle a \,\|\underline{T}^k\|\, a'\rangle = \left[\frac{(a+a'+k+1)!(a-a'-k)!(a'-a-k)!}{(a+a'-k)!}\right]^{\frac{1}{2}} \quad \text{(III.47)}$$

It will be noticed immediately that the matrix elements of $\frac{1}{r}$ cannot be calculated under this scheme, and this is a problem in all O(2,1) treatments of the harmonic oscillator. This problem does not arise in the hydrogen atom as the tensors there are all of integral k and the $k \to -(k+1)$ $k < 0$ transformation can be used without restriction. Thus matrix elements of r^{2k} $k \leqslant -1$ can be calculated, and a few examples are:

$$\langle N\ell|\frac{1}{r^2}|N\ell\rangle = \frac{2}{(2\ell+1)}$$

$$\langle N\ell|\frac{1}{r^4}|N\ell\rangle = \frac{4(2N+3)}{(2\ell-1)(2\ell+1)(2\ell+3)}$$

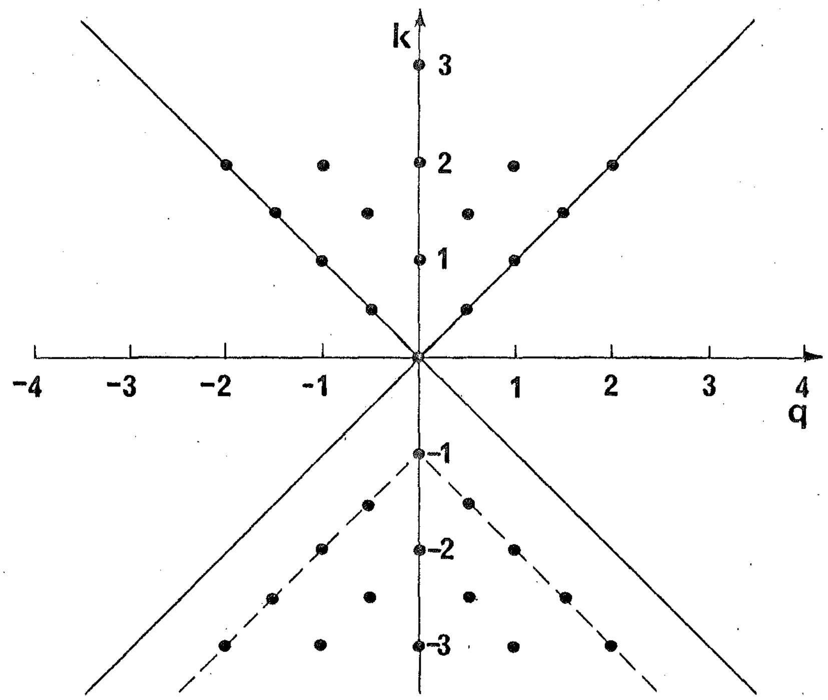
$\therefore$

$$\langle N+2\ \ \ell+2|\frac{1}{r^4}|N\ell\rangle = (-1)^{(N+\ell)/2}\ \frac{4[(N+\ell+1)(N+\ell+3)]^{\frac{1}{2}}}{(2\ell+5)(2\ell+3)(2\ell+1)}$$

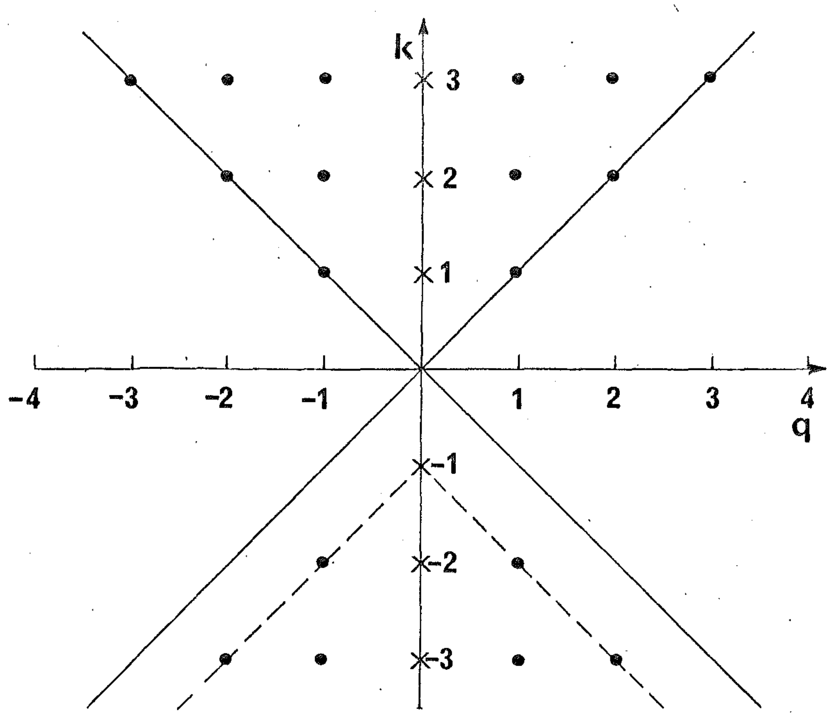
Matrix elements of the other r^{2k} operators may also be calculated in this manner. The following two figures show the tensors of the harmonic oscillator whose matrix elements can be calculated using the group O(2,1).

VII. Comparison with the Hydrogen Atom

As the variable of the harmonic oscillator radial wave-function does not contain N, no dilation operator is necessary as it is in the hydrogenic atom. The absence of the dilation operator simplifies the calculation of matrix elements off-diagonal in N. As off-diagonal matrix elements of the hydrogen atom have not yet been treated in the SO(3) × O(2,1)



The diagram of the T^k_q tensors that can be calculated using the O(2,1) scheme for the harmonic oscillator.



The dots represent the tensors of interest in the hydrogen atom problem. The crosses represent the matrix elements that have actually been calculated using the group O(2,1).

scheme the problem of the Clebsch-Gordan coefficients for $k < 0$ $|q| = |k|$ has not been considered. In the hydrogen atom only diagonal matrix elements $r^k = T_0^k$ have been considered explicitly and no problem arises with $\frac{1}{r}$ which transforms as T_0^{-1} and not as $T_{\pm\frac{1}{2}}^{-\frac{1}{2}}$ as in the harmonic oscillator.

VIII. Comparison with Armstrong's Scheme

Armstrong's[8] treatment of the harmonic oscillator problem introduced the 4th variable t so that his wavefunctions and operators are

$$f_{ab} = \left[\frac{\ell+\frac{1}{2}}{4\pi\beta^{\frac{1}{2}}}\right]^{\frac{1}{2}} e^{(n+\frac{1}{2})t/2}\ z^{\frac{1}{4}}\ R_{n\ell}(z)$$

and

$$k_{\pm} = e^{\pm it}\quad z\frac{d}{dz} \mp i\frac{\partial}{\partial t} \mp \frac{z}{2}$$

$$k_0 = i\frac{\partial}{\partial t}$$

At first study this introduction of t seemed somewhat artificial but on closer observation it is seen that t coincides with time. In the Schrodinger scheme the time dependence is factored off as follows[10]

$$\psi_{n\ell m}(r)\ e^{-i(2n+\ell+\frac{3}{2})t}$$

and the group generators are

$$k_{\pm} = \pm(z\frac{d}{dz} \mp \frac{z}{2} \pm \frac{H}{2} + \frac{3}{4})$$

$$k_0 = \tfrac{1}{2}H = \tfrac{1}{4}(P^2 + r^2).$$

To treat the time dependent case the $Y_{\ell m}(\theta\varphi)$ is time independent and can be factored off. The radial wavefunction is then written

$$R_{n\ell}(r)\ e^{-i(2n+\ell+\frac{3}{2})t}$$

and on carrying out the usual replacement of $\frac{1}{2}(P^2+r^2)$ by $i\frac{\partial}{\partial t}$ the operators

$$k_{\pm} = e^{\pm it}\ (z\frac{d}{dz} \mp i\frac{\partial}{\partial t} \mp \frac{z}{2})$$

$$k_0 = i\frac{\partial}{\partial t}$$

are obtained. Hence the two schemes are equivalent, one being the time independent scheme and the other being time dependent. There is little point in pursuing this topic further as it is well treated by Moshinsky, Kumei, Shibuya and Wulfman[10].

IX. Conclusion

It has been shown that it is possible to calculate the matrix elements of r^{2k} for harmonic oscillator wavefunctions using the algebra of the group O(2,1). The advantage of this method over that of integrating the radial matrix elements directly is that once the Clebsch-Gordan coefficients have been found they may be calculated from a standard summation for any value of ℓ, N, ℓ' and N' so that all of the difficulties of a long iteration process are bypassed.

The group Sp(6,R) is not the dynamical group of the harmonic oscillator[11,13] for while it contains both the degeneracy group SU(3) and the transition group SO(3) × O(2,1) it contains no operators acting between states such as $\langle N-1|$ and $|N\rangle$. The boson states split into two Sp(6,R) representations, one for even N and one for odd N. A group which has generators acting between states of odd and even N is proposed in the next chapter.

CHAPTER IV

NON-COMPACT DYNAMICAL GROUPS AND THE HARMONIC OSCILLATOR

I. Introduction

In the treatment of the harmonic oscillator several group schemes have been suggested[3,22]; the degeneracy group of the harmonic oscillator has been known for some time[3], but the dynamical group has proved more difficult to derive. The degeneracy group is SU(3) and this has been studied extensively in chapters one and two. The idea of extending SU(3) to SU(4) and SU(3,1) has been considered but this leads to the difficulty of forming a SU(4) generator which commutes with all of the generators of SU(3) and which does not involve taking square roots of the Hamiltonian[12]. An additional problem is that neither SU(4) nor SU(3,1) contains the transition group as a subgroup.

The group Sp(6,R) has been suggested[12], but the problem here is that two representations of it are required, one for N even and one for N odd[11,13]. The group proposed here is one which has a single representation that generates all of the states of the harmonic oscillator for both even and odd N. The proposed group is H_4 ×) SP(6,R) where Sp(6,R) is the six-dimensional real symplectic group and H_4 is the Heisenberg group in three dimensions. The symbol ×) implies semi-direct product and this will be defined later. The group H_4 ×) Sp(6,R) splits into two subgroups Sp(6,R) N even and Sp(6,R) N odd.

The subgroups H_4 ×) SU(3), H_2 ×) SO(3), H_4 ×) O(2,1) of the group H_4 ×) Sp(6,R) are also investigated. Finally, the group $H_4 \times) Sp(6,R)$ and its subgroups being contractions of larger groups is investigated.

II. Formation of the Dynamical Group

In order to form the dynamical group of the harmonic oscillator a group which contains the degeneracy group SU_3 is required. If the following boson operators a_x, a_y, a_z, $a_x^\dagger, a_y^\dagger, a_z^\dagger$ are defined in a Cartesian basis with the boson commutation relation

$$[a_\alpha a_\beta^\dagger] = -\delta(\alpha\beta) \tag{IV.1}$$

where α,β range over x, y and z. In order to generate a unitary group the following combination of operators is taken

$$T_{ij} = \tfrac{1}{2}(a_i^\dagger a_j + a_j a_i^\dagger)$$

where $i,j = x,y,z$; these operators can be shown to close on SU_3[3]. If we then add the operators $P_{ij} = \frac{1}{2}(a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger)$ and $Q_{ij} = \frac{1}{2}(a_i a_j + a_j a_i)$ these close under the commutation relations

$$\begin{aligned}
[T_{\alpha\beta}\ T_{\gamma\delta}] &= T_{\alpha\delta}\delta(\beta\gamma) - T_{\alpha\beta}\delta(\alpha\delta)\\
[T_{\alpha\beta}\ Q_{\gamma\delta}] &= -Q_{\delta\beta}\delta(\gamma\alpha) - Q_{\gamma\beta}\delta(\alpha\delta)\\
[T_{\alpha\beta}\ P_{\gamma\delta}] &= P_{\alpha\delta}\delta(\beta\gamma) + P_{\alpha\gamma}\delta(\beta\delta)\\
[P_{\alpha\beta}\ Q_{\gamma\delta}] &= -\{T_{\beta\gamma}\delta(\alpha\delta) + T_{\alpha\gamma}\delta(\beta\delta) + T_{\beta\delta}\delta(\alpha\gamma) + T_{\alpha\delta}\delta(\beta\gamma)\}\,.
\end{aligned} \tag{IV.2}$$

to form the albegra $Sp(6,R)$.

Now in order to complete the semidirect product group the following operators are added, a_x, a_y, a_z, $a_x^\dagger, a_y^\dagger, a_z^\dagger$ and the unit element E. The group now formed is $H_4 \times) Sp(6,R)$, with the commutation relations

$$
\begin{aligned}
[T_{\alpha\beta}\ a_{\gamma}] &= -a_{\beta}\delta(\alpha\gamma) \\
[T_{\alpha\beta}\ a_{\gamma}^{\dagger}] &= a_{\alpha}^{\dagger}\delta(\beta\gamma) \\
[Q_{\alpha\beta}\ a_{\gamma}^{\dagger}] &= a_{\alpha}\delta(\beta\gamma) + a_{\beta}\delta(\alpha\gamma) \\
[P_{\alpha\beta}\ a_{\gamma}] &= -a_{\alpha}^{\dagger}\delta(\beta\gamma) - a_{\beta}^{\dagger}\delta(\alpha\gamma) \\
[a_{\alpha}\ a_{\beta}^{\dagger}] &= +E\delta(\alpha\beta).
\end{aligned}
\qquad \text{(IV.3)}
$$

This group is a semidirect product because the commutator of a Sp(6,R) generator and a H_4 generator is not zero as it would be in a direct product case. Diagrammatically we have under commutation

	Sp(6,R) generators	H_4 generators
Sp(6,R) generators	Sp(6,R) generators	H_4 generators
H_4 generators	H_4 generators	H_4 generators

To put the whole group scheme on a physical basis in which angular momentum occurs naturally it is better at this point to go to spherical coordinates to avoid the introduction of complex transformations later on.

The spherical tensor operators are defined as follows[42]:

$$
\begin{aligned}
a^{\dagger}_{\pm 1} &= \mp \frac{1}{\sqrt{2}} (a^{\dagger}_{x} \pm i a^{\dagger}_{y}) \\
a_{\pm} &= \mp \frac{1}{\sqrt{2}} (a_{x} \pm i a_{y}) \\
a^{\dagger}_{0} &= a^{\dagger}_{z} \\
a_{0} &= a_{z}
\end{aligned} \tag{IV.4}
$$

These operators have the following relations under commutation with $ijk = \pm 1$ or 0, and $\delta(0) = 1$, $\delta(a) = 0$ where $a \neq 1$.

$$
\begin{aligned}
[a_k \; a_i a_j] &= 0 \\
[a_k \; a^{\dagger}_i a_j] &= (-1)^k \delta(k+1) a_j \\
[a_k \; a^{\dagger}_i a^{\dagger}_j] &= (-1)^k \delta(k+i) a^{\dagger}_j + (-1)^k \delta(k+j) a^{\dagger}_i \\
[a_k \; a_i a^{\dagger}_j] &= (-1)^k \delta(k+i) a_i \\
[a^{\dagger}_k \; a^{\dagger}_i a^{\dagger}_j] &= 0 \\
[a^{\dagger}_k \; a_i a^{\dagger}_j] &= (-1)^{i+1} \delta(1+k) a^{\dagger}_j \\
[a^{\dagger}_k \; a^{\dagger}_i a_j] &= (-1)^{j+1} \delta(k+j) a^{\dagger}_i \\
[a^{\dagger}_k \; a_i a_j] &= (-1)^{i+1} \delta(k+i) a_j + (-1)^{j+1} \delta(k+j) a_i \\
[a_i a_j \; a_k a_\ell] &= 0 \\
[a_i a_j \; a_k a^{\dagger}_\ell] &= (-1)^j \delta(\ell+j) a_k a_i + (-1)^i \delta(i+\ell) a_k a_j \\
[a_i a_j \; a^{\dagger}_k a_\ell] &= (-1)^i \delta(i+k) a_j a_\ell + (-1)^j \delta(k+j) a_i a_\ell \\
[a_i a_j \; a^{\dagger}_k a^{\dagger}_\ell] &= (-1)^j \Big(\delta(k+j) a_i a^{\dagger}_\ell + \delta(\ell+j) a_i a^{\dagger}_k \Big) \\
&\quad + (-1)^i \Big(\delta(k+i) a^{\dagger}_\ell a_j + \delta(i+\ell) a^{\dagger}_k a_\ell \Big) \\
[a^{\dagger}_i a_j \; a^{\dagger}_k a_\ell] &= (-1)^j \delta(k+j) a^{\dagger}_i a_\ell + (-1)^{i+1} \delta(\ell+i) a^{\dagger}_k a_j \\
[a^{\dagger}_i a_j \; a^{\dagger}_k a^{\dagger}_\ell] &= (-1)^j \Big(\delta(\ell+j) a^{\dagger}_i a^{\dagger}_k + \delta(k+j) a^{\dagger}_i a^{\dagger}_\ell \Big) \\
[a^{\dagger}_i a^{\dagger}_j \; a^{\dagger}_k a^{\dagger}_\ell] &= 0.
\end{aligned} \tag{IV.5}
$$

III. Sub-Group Structure

Observation of the above commutators leads one immediately to the formation of the explicit construction of the SU_3 group generators, namely:

$$B_0^{\,0} = \sqrt{\tfrac{2}{3}}\,(-a_1^\dagger a_{-1} + a_0^\dagger a_0 + a_{-1}^\dagger a_1)$$

With H the harmonic oscillator Hamiltonian being given by

$$H = \left(\sqrt{\tfrac{3}{2}}\,B_0^{\,0} + \tfrac{3}{2}\right)$$

this is a generator of U_3 but not of SU_3, so that the proper generators of SU_3 are

$$\begin{aligned}
L_0 &= B_1^{\,0} = (a_{-1}^\dagger a_1 + a_1^\dagger a_{-1}) \\
L_\pm &= B_1^{\pm 1} = (a_{\pm 1}^\dagger a_0 - a_0^\dagger a_{\pm 1}) \\
B_2^{\,0} &= \frac{-1}{\sqrt{3}}\,(2a_0^\dagger a_0 + a_1^\dagger a_1 + a_1^\dagger a_1) \qquad\qquad \text{(IV.6)} \\
B_2^{\pm 1} &= -(a_{\pm 1}^\dagger a_0 + a_0^\dagger a_{\pm 1}) \\
B_2^{\pm 2} &= -\sqrt{2}(a_{\pm 1}^\dagger a_{\pm 1})
\end{aligned}$$

Thus the degeneracy group chain $H_4 \times) \, Sp(6,R) \supset SU_3 \supset R_3 \supset R_2$ is formed and the states $|N\ell m\rangle$ of the harmonic oscillator are characterised by the eigenvalues of the operators L_0 of R_2, the Casimir operator L^2 of R_3, and H of U_3. The fact that these are the only quantum numbers required will arise naturally in the derivation of the matrix elements of $a_{\pm 1}$, $a_{\pm 1}^\dagger$, a_0, $a_0^\dagger$.

Now the operators B_λ^m obey the following commutation relations[45]

$$[B_\lambda^m \; B_{\lambda'}^{m'}] = -\sqrt{2} \sum_{\lambda''} \alpha(\lambda\lambda'\lambda'';mm')\; B_{\lambda''}^{m''} \qquad\qquad \text{(IV.7)}$$

where m" = m+m' and

$$\alpha(\lambda\lambda'\lambda''mm') = 2(-1)^{1+\lambda}[\lambda]^{\frac{1}{2}}[\lambda']^{\frac{1}{2}}\ C^{\lambda\lambda'\lambda''}_{mm'}W(\lambda 1\lambda''1;1\lambda') \qquad \text{(IV.8)}$$

where $[\lambda] = 2\lambda+1$, $C^{\lambda\lambda'\lambda''}_{mm'}$ is a Clebsch-Gordan coefficient and $W(\lambda 1\lambda''1;1\lambda')$ is a Racah coefficient which implies the condition $\lambda+\lambda'+\lambda''$ odd, otherwise $\alpha = 0$. Now $B^m_\mu|N\ell m\rangle$ changes ℓ by ± 2 or 0 and m by ± 2, ± 1 or 0. Since SU_3 is the degeneracy group it cannot change the value of N, i.e. it cannot couple different representations of SU_3. In order to get from one SU_3 representation to another a set of operators that change N are required. Consideration of the operators

$$\begin{aligned}
k_+ &= -\tfrac{1}{2}(a_0^\dagger a_0^\dagger - 2a_1^\dagger a_1^\dagger) \\
k_- &= -\tfrac{1}{2}(a_0 a_0 - 2a_0 a_{-1}) \\
k_0 &= \tfrac{1}{2}H = \tfrac{1}{2}\left(\sqrt{\tfrac{3}{2}}\ B_0{}^0 + \tfrac{3}{2}\right) \\
&= \tfrac{1}{2}(-a_1^\dagger a_{-1} - a_1^\dagger a_1 + a_0^\dagger a_0)
\end{aligned} \qquad \text{(IV.9)}$$

and the operators $L_\pm$ and L_0 lead to the <u>direct product</u> group $O(2,1) \times SO(3)$ with the commutation relations

$$\begin{aligned}
[k_+\ k_-] &= -2k_0 \\
[k_0\ k_\pm] &= \pm k_\pm \\
[L_+\ L_-] &= 2L_0 \\
[L_0\ L_\pm] &= L_\pm \\
[k_i\ L_j] &= 0 \quad \text{for all } i,j
\end{aligned} \qquad \text{(IV.10)}$$

i.e. diagrammatically

Commutation	k_+ k_- k_0	L_+ L_- L_0
k_+ k_- k_0	k type	zeros
L_+ L_- L_0	zeros	L type

Thus one can see by example the difference between a semi-direct product and a direct product. This $O(2,1) \times SO(3)$ group has been dealt with extensively in chapter 3.

IV. Determination of the Matrix Elements of the Group Generators $a_{\pm 1}$, a_0, $a^\dagger_{\pm 1}$, $a^\dagger_0$

In the derivation of the matrix elements of the operators $a_{\pm 1}$, a_0, $a^\dagger_{\pm 1}$, $a^\dagger_0$ the treatment of Louck[42] is followed closely, mainly because it can be generalised without difficulty to any dimension.

If the harmonic oscillator wavefunction is written

$$\psi(\lambda\ \ell_{n-1}, \ell_{n-2} \ldots \ell_1) = R(\lambda\ \ell_{n-1}) Y(\ell_{n-1} \ldots \ell_1) \qquad \text{(IV.11)}$$

where $R(\lambda\ \ell_{n-1})$ depends on the radial function r alone and $Y(\ell_{n-1} \ldots \ell_1)$ are the n-dimensional spherical harmonics. Now if the generalized spherical harmonics are separated off the radial equation becomes

$$H(\ell)\ R(\lambda\ell) = \lambda R(\lambda\ell) \qquad \text{(IV.12)}$$

where

$$H(\ell) = \tfrac{1}{2}\left[-\frac{d^2}{dr^2} - \frac{(n-1)}{r}\frac{d}{dr} + \frac{\ell(\ell+n-2)}{r^2} + r^2\right] \tag{IV.13}$$

where $\ell = \ell_{n-1}$, as the subscript is no longer needed, and n is the dimension of the oscillator.

Infeld and Hull[36] have considered the double factorization of the eigenvalue equation, but this is not enough for the present purposes, so a quadruple factorization is used. Following Louck[42] four operators are defined.

$$\begin{aligned}
\Omega^+(\ell) &= -\frac{d}{dr} + \frac{\ell}{r} + r \\
\Omega^-(\ell) &= \frac{d}{dr} + \frac{(\ell+n-2)}{r} + r \\
\omega^+(\ell) &= \frac{d}{dr} - \frac{\ell}{r} + r \\
\omega(\ell) &= -\frac{d}{dr} - \frac{(\ell+n-2)}{r} + r
\end{aligned} \tag{IV.14}$$

which satisfy the following relations

$$\begin{aligned}
2H(\ell) &= \Omega^-(\ell+1)\Omega^+(\ell) - 2\ell - n \\
2H(\ell) &= \Omega^+(\ell-1)\Omega^-(\ell) - 2\ell - n + 4 \\
2H(\ell) &= \omega^-(\ell+1)\omega^+(\ell) + 2\ell + n \\
2H(\ell) &= \omega^+(\ell-1)\omega^-(\ell) + 2\ell + n - 4
\end{aligned} \tag{IV.15}$$

By appropriate multiplication by $\Omega^{\pm}(\ell)$ and $\omega^{\pm}(\ell)$ one obtains

$$\begin{aligned}
H(\ell+1)\Omega^+(\ell) - \Omega^+(\ell)H(\ell) &= \Omega^+(\ell) \\
H(\ell-1)\Omega^-(\ell) - \Omega^-(\ell)H(\ell) &= -\Omega^-(\ell) \\
H(\ell+1)\omega^+(\ell) - \omega^+(\ell)H(\ell) &= -\omega^+(\ell) \\
H(\ell-1)\omega^-(\ell) - \omega^-(\ell)H(\ell) &= \omega^-(\ell)
\end{aligned} \tag{IV.16}$$

Operating on the radial wavefunction $R(\lambda\ell)$ with each of these equations leads to

$$H(\ell\pm1)\Omega^{\pm}(\ell)R(\lambda\ell) = (\lambda\pm1)\Omega^{\pm}(\ell)R(\lambda\ell) \tag{IV.17}$$

$$H(\ell\pm1)\omega^{\pm}(\ell)R(\lambda\ell) = (\lambda\mp1)\omega^{\pm}(\ell)R(\lambda\ell) \tag{IV.18}$$

which implies

$$\Omega^{\pm}(\ell)R(\lambda\ell) = N^{\pm}(\lambda\ell)R(\lambda\pm1,\ell\pm1) \tag{IV.19}$$

$$\omega^{\pm}(\ell)R(\lambda\ell) = M^{\pm}(\lambda\ell)R(\lambda\mp1,\ell\pm1) \tag{IV.20}$$

where $N^{\pm}(\lambda\ell)$ and $M^{\pm}(\lambda\ell)$ are normalizing coefficients. It can be shown that the operators

$$\omega^{+}(\ell+1)\Omega^{+}(\ell) \qquad \text{and} \qquad \omega^{-}(\ell+1)\Omega^{-}(\ell)$$

are equal to the operators

$$\Omega^{+}(\ell+1)\omega^{+}(\ell) \qquad \text{and} \qquad \Omega^{-}(\ell+1)\omega^{-}(\ell)$$

respectively.

If one substitutes $\ell+1$ for ℓ in equation (16,C) and multiplies on the right by $\Omega^{+}(\ell)$ one obtains

$$H(\ell+2)\omega^{+}(\ell+1)\Omega^{+}(\ell) - \omega^{+}(\ell+1)H(\ell+1)\Omega^{+}(\ell)$$

$$= \omega^{+}(\ell+1)\Omega^{+}(\ell) \tag{IV.22}$$

while the result

$$\omega^{+}(\ell+1)H(\ell+1)\Omega^{+}(\ell) - \omega^{+}(\ell+1)\Omega^{+}(\ell)H(\ell)$$

$$= \omega^{+}(\ell+1)\Omega^{+}(\ell) \tag{IV.23}$$

is obtained in a similar fashion. Addition of 22 and 23 gives

$$H(\ell+2)\omega^{+}(\ell+1)\Omega^{+}(\ell) = \omega^{+}(\ell+1)\Omega^{+}(\ell)H(\ell) \tag{IV.24}$$

Similarly

$$H(\ell-2)\omega^-(\ell-1)\Omega^-(\ell) = \omega^-(\ell-1)\Omega^-(\ell)H(\ell) \qquad \text{(IV.25)}$$

Operating on $R(\lambda\ell)$ gives

$$H(\ell+2)\{\omega^+(\ell+1)\Omega^+(\ell)R(\lambda\ell)\} = \lambda\{\omega^+(\ell+1)\Omega^+(\ell)R(\lambda\ell)\}$$

$$H(\ell-2)\{\omega^-(\ell-1)\Omega^-(\ell)R(\lambda\ell)\} = \lambda\{\omega^-(\ell-1)\Omega^-(\ell)R(\lambda\ell)\} \qquad \text{(IV.26)}$$

so that if $R(\lambda\ell)$ is a solution of

$$H(\ell)R(\lambda\ell) = \lambda R(\lambda\ell)$$

then $\omega^+(\ell+1)\Omega^+(\ell)R(\lambda\ell)$ and $\omega^-(\ell+1)\Omega^-(\ell)R(\lambda\ell)$ are solutions corresponding to the same λ but to $\ell\pm2$ respectively. A general relation of the following form is found by iteration

$$\omega^+(\ell+2k+1)\Omega^+(\ell+2k)\omega^+(\ell+2k-1)\Omega^+(\ell+2k-2) \ldots \Omega^+(\ell)R(\lambda\ell) \qquad \text{(IV.26)}$$

and

$$\omega^-(\ell-2k-1)\Omega^-(\ell-2k)\omega^-(\ell-2k+1)\Omega^-(\ell-2k+2) \ldots \omega^-(\ell-1)\Omega^-(\ell)R(\lambda\ell) \qquad \text{(IV.28)}$$

where $k = 0,1,2 \ldots$ are solutions of

$$H(\ell)R(\lambda\ell) = \lambda R(\lambda\ell)$$

corresponding to the same λ but to different ℓ values

$\ell+2, \ell+4 \ldots \ell+2k+2;\ \ell-2, \ell-4 \ldots \ell-2k+2$ respectively.

It is already known from the theory of spherical harmonics that a lower bound $\ell = 0$ exists, and that ℓ may be chosen from $0,1,2,\ldots.$ It will be shown later that for a given λ there also exists an upper bound for ℓ.

V. Determination of the Normalization Coefficients

To determine the relation between $N^-(\lambda\ell)$, $N^+(\lambda\ell)$ and $M^-(\lambda\ell)$, $M^+(\lambda\ell)$ one must return to the general n dimensional notation. Firstly from the theory of generalised spherical harmonics, the following operators may be derived

$$\gamma^+_{n-1}(\ell_{n-1})Y(\ell_{n-1} \dots \ell_1)$$

$$= \left[\frac{(2\ell_{n-1}+n-2)(\ell_{n-1}-\ell_{n-1}+1)(\ell_{n-1}-\ell_{n-2}+n-2)}{(2\ell_{n-1}+n)}\right]^{\frac{1}{2}}$$

$$\times\ Y(\ell_{n-1}+1, \ell_{n-2} \dots \ell_1) \tag{IV.29}$$

$$\gamma^-_{n-1}(\ell_{n-1})Y(\ell_{n-1} \dots \ell_1)$$

$$= \left[\frac{(2\ell_{n-1}+n-2)(\ell_{n-1}-\ell_{n-2})(\ell_{n-1}+\ell_{n-2}+n-3)}{(2\ell_{n-1}+n-4)}\right]^{\frac{1}{2}}$$

$$\times\ Y(\ell_{n-1}-1, \dots \ell_1) \tag{IV.30}$$

Now the following operations may be performed

$$\Omega^+(\ell_{n-1})\gamma^+_{n-1}(\ell_{n-1})\psi(\lambda\ell_{n-1},\dots,\ell_1)$$

$$= N^+(\lambda\ell_{n-1})\left[\frac{(2\ell_{n-1}+n-2)(\ell_{n-1}-\ell_{n-2}+1)(\ell_{n-1}+\ell_{n-2}+n-2)}{(2\ell_{n-1}+n)}\right]^{\frac{1}{2}}$$

$$\times\ \psi(\lambda, \ell_{n-1}+1 \dots \ell_1) \tag{IV.31}$$

$$\Omega^-(\ell_{n-1})\gamma^-(\ell_{n-1})Y(\lambda, \ell_{n-1} \dots \ell_1)$$

$$= N^-(\lambda\ell)\left[\frac{(2\ell_{n-1}+n-2)(\ell_{n-1}-\ell_{n-2})(\ell_{n-1}+\ell_{n-2}+n-3)}{(2\ell_{n-1}+n-4)}\right]^{\frac{1}{2}}$$

$$\times\ \psi(\lambda, \ell_{n-1}-1 \dots \ell_1) \tag{IV.32}$$

$$\omega^{+}(\ell_{n-1})\gamma^{+}(\ell_{n-1})\ (\lambda,\ell_{n-1}\ \dots\ \ell_1)$$

$$= M^{+}(\lambda,\ell_{n-1})\left[\frac{(2\ell_{n-1}+n-2)(\ell_{n-1}+\ell_{n-2}+1)(\ell_{n-1}+\ell_{n-2}+n-2)}{(2\ell_{n-1}+n)}\right]^{\frac{1}{2}}$$

$$\times\ \psi(\lambda,\ell_{n-1}+1\ \dots\ \ell_1) \tag{IV.33}$$

$$\omega^{-}(\ell_{n-1})\gamma^{-}(\ell_{n-1})\psi(\lambda,\ell_{n-1}\ \dots\ \ell_1)$$

$$= M^{-}(\lambda\ell_{n-1})\left[\frac{(2\ell_{n-1}+n-2)(\ell_{n-1}-\ell_{n-2})(\ell_{n-1}+\ell_{n-2}+n-3)}{2\ell_{n-1}+n-4}\right]^{\frac{1}{2}}$$

$$\times\ \psi(\lambda,\ell_{n-1}-1\ \dots\ \ell_1) \tag{IV.34}$$

Now

$$\alpha_n = P_n + i\chi_n = \frac{i}{2\ell_{n-1}+n-2}$$

$$\times\ [\Omega^{+}(\ell_{n-1})\gamma^{+}_{n-1}(\ell_{n-1}) + \omega^{-}(\ell_{n-1})\gamma^{-}_{n-1}(\ell_{n-1})] \tag{IV.35}$$

$$\beta_n = P_n - i\chi_n = \frac{-i}{(2\ell_{n-1}+n-2)}$$

$$\times\ [\omega^{+}(\ell_{n-1})\gamma^{+}_{n-1}(\ell_{n-1}) + \Omega^{-}(\ell_{n-1})\gamma^{-}_{n-1}(\ell_{n-1})] \tag{IV.36}$$

This can be easily verified when one considers the following

$$\chi_j = r\cos\theta_{j-1}\sin\theta_j\sin\theta_{j+1}\ \dots\ \sin\theta_{n+1} \tag{IV.37}$$

and

$$P_n = -i\left[\cos\theta_{n-1}\frac{\partial}{\partial r} - \frac{\sin\theta_{n-1}}{r}\frac{\partial}{\partial\theta_{n-1}}\right],\quad n \geqslant 3 \tag{IV.38}$$

Note that α_n and β_n are conjugate operators which when operating on $\psi(\lambda\ell_{n-1}\ \dots\ \ell_1)$ with each of α and β lead to the result

$$(\lambda+1,\ell_{n-1}+1\ \dots\ \ell_1|\alpha_n|\lambda,\ell_{n-1}\ \dots\ \ell_1)$$

$$= (\lambda,\ell_{n-1}\ \dots\ \ell_1|\beta_n|\lambda+1,\ell_{n-1}+1\ \dots\ \ell_1)^{*} \tag{IV.39}$$

from which

$$N^+(\lambda,\ell_{n-1}) = [N^-(\lambda+1,\ell_{n-1}+1)]^* \qquad \text{(IV.40)}$$

and $$M^-(\lambda,\ell_{n-1}) = [M^+(\lambda+1,\ell_{n-1}-1)]^* \qquad \text{(IV.41)}$$

are obtained. From eqns (IV.15b), (IV.15c), (IV.19) and (IV.20), and the above equations (IV.40) and (IV.41),

$$H(\ell)k(\lambda\ell) = \lambda R(\lambda\ell) = \tfrac{1}{2}\{|N^-(\lambda\ell)|^2 - 2\ell - n + 4\}R(\lambda\ell) \qquad \text{(IV.42)}$$

$$H(\ell)R(\lambda\ell) = \lambda R(\lambda\ell) = \tfrac{1}{2}\{|M^+(\lambda\ell)|^2 + 2\ell + n\}R(\lambda\ell) \qquad \text{(IV.43)}$$

where here $\ell = \ell_{n-1}$. Add (42) and (43) to get

$$\lambda = \tfrac{1}{4}|N^-(\lambda\ell)|^2 + \tfrac{1}{4}|M^+(\lambda\ell)|^2 + 1 \geqslant 1 \qquad \text{(IV.44)}$$

Similarly

$$\lambda - \ell - \tfrac{n}{2} = \tfrac{1}{2}|M^+(\lambda\ell)|^2 \geqslant 0 \qquad \text{(IV.45)}$$

From equations (44) and (45) for a given value of λ there exists a maximum value ℓ' of ℓ such that $R(\lambda\ell) \neq 0$ while $R(\lambda-1,\ell'+1) = 0$. Hence

$$\omega^+(\ell')R(\lambda\ell') = 0 \qquad \text{(IV.46)}$$

Operating on $R(\lambda\ell')$ with equation (IV.15c) leads directly to the result

$$H(\ell')R(\lambda\ell') = \lambda R(\lambda\ell') = (\ell' + \tfrac{n}{2})\, R(\lambda\ell') \qquad \text{(IV.47)}$$

and hence

$$\lambda = \ell' + \tfrac{n}{2}. \qquad \text{(IV.48)}$$

Denote ℓ' by N so that

$$H\psi(N\ \ell_{n-1} \dots \ell_1) = (N + \tfrac{n}{2})\psi(\ell_{n-1} \dots \ell_1) \qquad \text{(IV.49)}$$

is obtained where here N is integral since ℓ' is integral and

$\ell'_{mn} = 0$ allows N to take the values of 0 1 2 3 .... For a given N ℓ may take the values N, N-2, N-4 ... 1 or 0.

The normalization requirement

$$\int \psi^*(\lambda', \ell'_{n-1} \ldots \ell'_1)\psi(\lambda, \ell_{n-1} \ldots \ell_1)dV$$
$$= \delta_{\lambda'\lambda} \prod_{i=1}^{n-1} \delta(\ell_i' \ell_i) \tag{IV.50}$$

where $\int dV = \int r^{n-1} dr d\omega$ requires the $R(N\ell)$ functions to be normalizable which in turn implies $\Omega^{\pm}(\ell)R(N\ell)$ and $\omega^{\pm}(\ell)R(N\ell)$ are either normalizable or zero.

<u>Evaluation of the Normalization Coefficients</u>

To evaluate the normalization coefficients, substitute $\lambda = (N + \frac{n}{2})$ into (IV.45) and (IV.44) to obtain

$$M^+(N\ell) = [2(N-\ell)]^{\frac{1}{2}} \tag{IV.51}$$

$$N^+(N\ell) = -[2(N+\ell+n-2)]^{\frac{1}{2}} \tag{IV.52}$$

and using (40) and (41) gives

$$N^+(N\ell) = -[2(N+\ell+n)]^{\frac{1}{2}} \tag{IV.53}$$

$$M^-(N\ell) = [2(N-\ell+2)]^{\frac{1}{2}} \tag{IV.54}$$

where $N^{\pm}(\lambda\ell)$ and $M^{\pm}(\lambda\ell)$ are denoted by $N^{\pm}(N\ell)$ and $M^{\pm}(N\ell)$ respectively, with an appropriate choice of phase. Hence (19) and (20) become

$$\Omega^+(\ell) = -[2(N+\ell+n)]^{\frac{1}{2}} R(N+1 \;\; \ell+1) \tag{IV.55}$$

$$\Omega^-(\ell) = -[2(N+\ell+n-2)]^{\frac{1}{2}} R(N-1 \;\; \ell-1) \tag{IV.56}$$

$$\omega^+(\ell) = [2(N-\ell)]^{\frac{1}{2}} R(N-1 \;\; \ell+1) \tag{IV.57}$$

$$\omega^-(\ell) = [2(N-\ell+2)]^{\frac{1}{2}} R(N+1 \;\; \ell-1) \tag{IV.58}$$

Thus in the general notation

$$\alpha_n\psi(N\ \ell_{n-1}\ \dots\ \ell_1)$$
$$= -i[2(N+\ell_{n-1}+n)]^{\frac{1}{2}}\left[\frac{(\ell_{n-1}-\ell_{n-2}+1)(\ell_{n-1}+\ell_{n-2}+n-2)}{(2\ell_{n-1}+n-2)(2\ell_{n-1}+n)}\right]^{\frac{1}{2}}$$
$$\times\ \psi(N+1,\ell_{n-1}+1\ \dots\ \ell_1)\ +\ i[2(N-\ell_{n-1}+2]^{\frac{1}{2}}$$
$$\times\left[\frac{(\ell_{n-1}-\ell_{n-2})(\ell_{n-1}+\ell_{n-2}+n-3)}{(2\ell_{n-1}+n-2)(2\ell_{n-1}+n-4)}\right]^{\frac{1}{2}}\psi(N+1,\ell_{n-1}-1\ \dots\ \ell_1). \qquad \text{(IV.59)}$$

$$\beta_n\psi(N,\ell_{n-1}\ \dots\ \ell_1)$$
$$= -i[2(N-\ell)]^{\frac{1}{2}}\left[\frac{(\ell_{n-1}-\ell_{n-2}+1)(\ell_{n-1}+\ell_{n-2}+n-2)}{(2\ell_{n-1}+n-2)(2\ell_{n-1}+n)}\right]^{\frac{1}{2}}$$
$$\times\ \psi(N-1,\ell_{n-1}+1\ \dots\ \ell_1)\ +\ i[2(N+\ell_{n-2}+n-2)]^{\frac{1}{2}}$$
$$\times\left[\frac{(\ell_{n-1}+\ell_{n-2})(\ell_{n-1}+\ell_{n-2}+n-3)}{(2\ell_{n-1}+n-2)(2\ell_{n-1}+n-4)}\right]^{\frac{1}{2}}\psi(N-1,\ell_{n-1}-1\ \dots\ \ell_1) \qquad \text{(IV.60)}$$

Since the ψ's are orthonormal the equations give the non-vanishing matrix elements of α_n and β_n.

Now $\alpha_j = P_j + ix_j$ (IV.61)

$$\beta_j = P_j - ix_j \qquad \text{(IV.62)}$$

For the three-dimensional harmonic oscillator the following identifications are made

$$\alpha_1 = \alpha_x = P_x + ix$$
$$\alpha_2 = \alpha_y = P_y + iy. \qquad \text{(IV.63)}$$
$$\alpha_3 = \alpha_z = P_z + iz$$

$$\beta_1 = \beta_x = P_x - ix$$
$$\beta_2 = \beta_y = P_y - iy \qquad \text{(IV.64)}$$
$$\beta_3 = \beta_z = P_z - iz.$$

On comparison with equations (IV.4), noting that

$$a_x = \frac{1}{\sqrt{2}}(x + iP_x)$$
$$a_x^\dagger = \frac{1}{\sqrt{2}}(x - iP_x) \qquad \text{(IV.65)}$$

the following relations are obtained:

$$a_{\pm 1}^\dagger = \pm \tfrac{1}{2}(\alpha_1 \pm i\alpha_2) \qquad \text{(IV.66)}$$

$$a_{\pm 1} = \mp \tfrac{1}{2}(\beta_1 \pm i\beta_2) \qquad \text{(IV.67)}$$

$$a_0^\dagger = \frac{-i\alpha_3}{\sqrt{2}} \qquad \text{(IV.68)}$$

$$a_0 = \frac{i\beta_3}{\sqrt{2}} \qquad \text{(IV.69)}$$

On substituting $\phi(N\ \ell_{n-1}\ \ldots\ \ell_1) = |N\ell m\rangle$ (IV.70)

for the three dimensional case, the operators of equations 66, 67, 68, 69 have the matrix elements

$$a_{\pm 1}^\dagger |N\ell m\rangle = -\frac{[N+\ell+3]^{\frac{1}{2}}}{\sqrt{2}} \left[\frac{(\ell\pm m+1)(\ell\pm m+2)}{(2\ell+1)(2\ell+3)}\right]^{\frac{1}{2}} |N+1, \ell+1, m\pm 1\rangle$$
$$-\frac{[N-\ell+2]^{\frac{1}{2}}}{\sqrt{2}} \left[\frac{(\ell\mp m)(\ell\mp m-1)}{(2\ell+1)(2\ell-1)}\right]^{\frac{1}{2}} |N+1, \ell-1, m\pm 1\rangle \qquad \text{(IV.71)}$$

$$a_{\pm 1} |N\ell m\rangle = +\left[\frac{N-\ell}{2}\right]^{\frac{1}{2}} \left[\frac{(\ell\pm m+1)(\ell\pm m+2)}{(2\ell+1)(2\ell+3)}\right]^{\frac{1}{2}} |N-1, \ell+1, m\pm 1\rangle$$
$$+\left[\frac{N+\ell+1}{2}\right]^{\frac{1}{2}} \left[\frac{(\ell\mp m)(\ell\mp m-1)}{(2\ell+1)(2\ell-1)}\right]^{\frac{1}{2}} |N-1, \ell-1, m\pm 1\rangle \qquad \text{(IV.72)}$$

$$a_0^\dagger |N\ell m\rangle = -[N+\ell+3]^{\frac{1}{2}} \left[\frac{(\ell-m+1)(\ell+m+1)}{(2\ell+1)(2\ell+3)}\right]^{\frac{1}{2}} |N+1, \ell+1, m\rangle$$
$$+ [N-\ell+2]^{\frac{1}{2}} \left[\frac{(\ell-m)(\ell+m)}{(2\ell+1)(2\ell-1)}\right]^{\frac{1}{2}} |N+1, \ell-1, m\rangle \qquad \text{(IV.73)}$$

$$a_0|N\ell m\rangle = +[N-\ell]^{\frac{1}{2}}\left[\frac{(\ell-m+1)(\ell+m+1)}{(2\ell+1)(2\ell+3)}\right]^{\frac{1}{2}}|N-1,\ell+1,m\rangle$$

$$- [N+\ell+1]^{\frac{1}{2}}\left[\frac{(\ell-m)(\ell+m)}{(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N-1,\ell-1,m\rangle \qquad \text{(IV.74)}$$

As all of the generators of the group $H_4 \times) Sp(6,R)$ can be constructed from products of $a^\dagger_{\pm 1}$, $a_{\pm 1}$, $a^\dagger_0$ and a_0 all of the matrix elements of the $H_4 \times) Sp(6,R)$ can be calculated from products of $a^\dagger_{\pm 1}$, $a_{\pm 1}$, $a^\dagger_0$ and a_o as follows, e.g.

$$L_0 = B_1{}^0 = a^\dagger_{-1}a_1 - a^\dagger_1 a_{-1} \qquad \text{(IV·75)}$$

Let $B_1{}^0$ operate on $|N\ell m\rangle$ to give

$$a^\dagger_{-1}a_1|N\ell m\rangle - a^\dagger_1 a_{-1}|N\ell m\rangle$$

which leads to

$$\left[\frac{N-\ell}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell+m+1)(\ell+m+2)}{(2\ell+1)(2\ell+3)}\right]^{\frac{1}{2}}\Big\{-\left[\frac{N+\ell+3}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell-m+1)(\ell-m+2)}{(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N\ \ \ell+2\ \ m\rangle$$

$$-\left[\frac{N-\ell}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell+m+2)(\ell+m+1)}{(2\ell+1)(2\ell+3)}\right]^{\frac{1}{2}}|N\ell m\rangle\Big\} + \left[\frac{N+\ell+1}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell-m)(\ell-m-1)}{(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}$$

$$\times\Big\{-\left[\frac{N+\ell+1}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell-m)(\ell-m-1)}{(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N\ell m\rangle - \left[\frac{N-\ell+2}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell+m)(\ell+m-1)}{(2\ell-1)(2\ell-3)}\right]^{\frac{1}{2}}$$

$$\times\ |N\ \ \ell-2\ \ m\rangle\Big\} - \left[\frac{N-\ell}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell-m+1)(\ell-m+2)}{(2\ell+1)(2\ell+3)}\right]^{\frac{1}{2}}\Big\{-\left[\frac{N+\ell+3}{2}\right]^{\frac{1}{2}}$$

$$\times\left[\frac{(\ell+m+1)(\ell+m+2)}{(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N\ \ \ell+2\ \ m\rangle - \left[\frac{N-\ell}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell-m+2)(\ell-m+1)}{(2\ell+3)(2\ell+1)}\right]^{\frac{1}{2}}|N\ell m\rangle\Big\}$$

$$-\left[\frac{N+\ell+1}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell+m)(\ell+m-1)}{(2\ell+1)(2\ell-1)}\right]^{\frac{1}{2}}\Big\{-\left[\frac{N+\ell+1}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell+m-1)(\ell+m)}{(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N\ell m\rangle$$

$$-\left[\frac{N-\ell+2}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell-m)(\ell-m-1)}{(2\ell-1)(2\ell-3)}\right]|N\ \ \ell-2\ \ m\rangle\Big\}$$

which simplifies down to $m|N\ell m\rangle$ so

$$L_0|N\ell m\rangle = m|NLm\rangle. \qquad \text{(IV.76)}$$

This is just what is expected as the eigenvalue of the sole R_2 generator. L_0 can also be labelled as $T^{(11)}_{10}$. The reason for this type of labelling will become clear later on. The R_3 generators are

$$B_1^{\pm} = T^{(11)}_{1\pm 1} = L_{\pm}|N\ell m\rangle = \frac{1}{\sqrt{2}}(\ell\mp m)(\ell\pm m+1)|N\ell m\pm 1\rangle \tag{IV.77}$$

The generators of SU_3 have matrix elements

$$B_2{}^{0}|N\ell m\rangle = T^{(11)}_{20}|N\ell m\rangle = (2N+3)\frac{(3m^2-\ell(\ell+1))}{(2\ell-1)(2\ell+3)}|N\ell m\rangle$$

$$+\ 3\left[\frac{(N-\ell)(N+\ell+3)(\ell-m+1)(\ell-m+2)(\ell+m+1)(\ell+m+2)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N\ \ell+2\ m\rangle$$

$$+\ 3\left[\frac{(N-\ell+2)(N+\ell+1)(\ell-m)(\ell+m)(\ell+m-1)(\ell-m-1)}{(2\ell-3)(2\ell-1)(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N\ \ell-2\ m\rangle \tag{IV.78}$$

$$B_2^{\pm 1}|N\ell m\rangle = T^{(11)}_{2\ 1}|N\ell m\rangle$$

$$= -\frac{(2N+3)(\pm 2m+1)}{(2\ell-1)(2\ell+3)}\left[\frac{(\ell\mp m)(\ell\pm m+1)}{2}\right]^{\frac{1}{2}}|N\ \ell\ m\pm 1\rangle$$

$$+\ [2(N-\ell)(N+\ell+3)]^{\frac{1}{2}}\left[\frac{(\ell+m+1)(\ell-m+1)(\ell\pm m+2)(\ell\pm m+3)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N\ \ell+2\ m\pm 1\rangle$$

$$-\ [2(N-\ell+2)(N+\ell+1)]^{\frac{1}{2}}\left[\frac{(\ell+m)(\ell-m)(\ell\mp m-1)(\ell\mp m+2)}{(2\ell-3)(2\ell-1)(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N\ \ell-2\ m\pm 1\rangle. \tag{IV.79}$$

$$B_2^{\pm 2}|N\ell m\rangle = T^{(11)}_{2\pm 2}|N\ell m\rangle$$

$$= \frac{(2N+3)}{(2\ell-1)(2\ell+3)}\left[\frac{(\ell\pm m+1)(\ell\pm m+2)(\ell\mp m)(\ell\mp m-1)}{2}\right]^{\frac{1}{2}}|N\ \ell\ m\pm 2\rangle$$

$$+\left[\frac{(N-\ell)(N+\ell+3)}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell\pm m+1)(\ell\pm m+2)(\ell\pm m+3)(\ell\pm m+4)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N\ \ell+2\ m+2\rangle$$

$$+\left[\frac{(N-\ell-2)(N+\ell+1)}{2}\right]^{\frac{1}{2}}\left[\frac{(\ell\mp m)(\ell\mp m+1)(\ell\mp m+2)(\ell\mp m+3)}{(2\ell-3)(2\ell-1)(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N\ \ell-2\ m\pm 2\rangle. \tag{IV.80}$$

Here the phase relationship between the coefficients of $|N\ell m\rangle$ and $|N\ \ell{\pm}2\ m\rangle$ has been fixed by the method of derivation of the operators $a^{\dagger}_{\pm 1}$, $a_{\pm 1}$, $a^{\dagger}_{0}$, a_{0}. The phase here is found to agree with that chosen in chapter 2. The arbitrary phase choice of Elliott arises from the necessity to take square roots in his derivation of the matrix elements of the group generators.

The O(2,1) generators are

$$k_0 = \tfrac{1}{2}H = \tfrac{1}{2}\,T^{(00)}_{00}\,|N\ell m\rangle$$

$$= (N + \tfrac{3}{2})\,|N\ell m\rangle \qquad \text{(IV.81)}$$

$$k_+|N\ell m\rangle = T^{(20)}_{00}|N\ell m\rangle$$

$$= \tfrac{1}{2}[(N+\ell+3)(N-\ell+2)]^{\frac{1}{2}}\,|N+2\ \ell\ m\rangle \qquad \text{(IV.82)}$$

$$k_-|N\ell m\rangle = T^{(02)}_{00}|N\ell m\rangle$$

$$= \tfrac{1}{2}[(N+\ell+1)(N-\ell)]^{\frac{1}{2}}\,|N-2\ \ell\ m\rangle. \qquad \text{(IV.83)}$$

The remaining group generators and their matrix elements are:

$$S^{(02)}_{20}|N\ell m\rangle = -[(N-\ell)(N+\ell+1)]^{\frac{1}{2}}\ \frac{[\ell(\ell+1)-3m^2]}{(2\ell-1)(2\ell+3)}\ |N-2\ \ell\ m\rangle$$

$$+\ \frac{3}{2}\ [(N-\ell)(N-\ell-2)]^{\frac{1}{2}}\left[\frac{(\ell-m+1)(\ell+m+1)(\ell-m+2)(\ell+m+2)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N-2\ \ell+2\ m\rangle$$

$$+\ \frac{3}{2}\ [(N+\ell+1)(N+\ell-1)]^{\frac{1}{2}}\left[\frac{(\ell-m+2)(\ell-m+1)(\ell+m)(\ell+m-1)}{(2\ell-3)(2\ell-1)(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N-2\ \ell-2\ m\rangle$$

(IV.84)

$$S^{(02)}_{2\pm1}|N\ell m\rangle = \mp[(N+\ell+1)(N-\ell)]^{\frac{1}{2}}\left[\frac{(\ell\mp m)(\ell+m+1)}{2}\right]^{\frac{1}{2}}\left[\frac{2m\pm1}{(2\ell-1)(2\ell+3)}\right]$$

$$|N-2\ \ell\ \ m\pm1\rangle$$

$$+\ [(N-\ell)(N-\ell-2)]^{\frac{1}{2}}\left[\frac{(\ell+m+1)(\ell-m+1)(\ell\pm m+2)(\ell\pm m+3)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N-2\ \ \ell+2\ \ m\pm1\rangle$$

$$-\ [(N+\ell+1)(N+\ell-1)]^{\frac{1}{2}}\left[\frac{(\ell-m)(\ell+m)(\ell\mp m-1)(\ell\mp m-2)}{(2\ell-3)(2\ell-1)(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N-2\ \ \ell-2\ \ m\pm1\rangle \tag{IV.85}$$

$$S^{(02)}_{2\pm2}|N\ell m\rangle$$

$$=\ [(N-\ell)(N+\ell+1)]^{\frac{1}{2}}\left[\frac{(\ell\mp m)(\ell\mp m-1)(\ell\pm m+1)(\ell\pm m+2)}{(2\ell-1)(2\ell-1)(2\ell+3)(2\ell+3)}\right]^{\frac{1}{2}}|N-2\ \ \ell\ \ m\pm2\rangle$$

$$+\ \left[\frac{(N-\ell)(N-\ell-2)}{4}\right]^{\frac{1}{2}}\left[\frac{(\ell\pm m+1)(\ell\pm m+2)(\ell\pm m+3)(\ell\pm m+4)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N-2\ \ \ell+1\ \ m\pm2\rangle$$

$$+\ \left[\frac{(N+\ell+1)(N+\ell-1)}{4}\right]^{\frac{1}{2}}\left[\frac{(\ell\mp m)(\ell\mp m-1)(\ell\mp m-2)(\ell\mp m-3)}{(2\ell-3)(2\ell-1)(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N-2\ \ \ell-2\ \ m\pm2\rangle \tag{IV.86}$$

$$S^{(20)}_{20}|N\ell m\rangle$$

$$= -[(N+\ell+3)(N-\ell+2)]^{\frac{1}{2}}\left[\frac{\ell(\ell+1)-3m^2}{(2\ell-1)(2\ell+3)}\right]|N+2\ \ \ell\ \ m\rangle$$

$$+\ \frac{3}{2}[(N-\ell+2)(N-\ell+4)]^{\frac{1}{2}}\left[\frac{(\ell-m)(\ell+m)(\ell-m-1)(\ell+m+1)}{(2\ell-3)(2\ell-1)(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N+2\ \ \ \ell-2\ \ m\rangle$$

$$+\ \frac{3}{2}[(N+\ell+3)(N+\ell+5)]^{\frac{1}{2}}\left[\frac{(\ell-m+1)(\ell+m+1)(\ell-m+2)(\ell+m+2)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N-2\ \ \ell+2\ \ m\rangle \tag{IV.87}$$

$$S^{(20)}_{2\pm1}|N\ell m\rangle =$$

$$\mp\ \frac{1}{2}[(N+\ell+3)(N-\ell+2)]^{\frac{1}{2}}[(\ell\mp m)(\ell\pm m+1)]^{\frac{1}{2}}\left[\frac{1\pm2m}{(2\ell-1)(2\ell+3)}\right]^{\frac{1}{2}}|N+2\ \ \ell\ \ m\pm1\rangle$$

$$+\ \frac{1}{2}[(N+\ell+3)(N+\ell+5)]^{\frac{1}{2}}\left[\frac{(\ell-m+1)(\ell+m+1)(\ell\pm m+2)(\ell\pm m+3)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N+2\ \ \ell+2\ \ m\pm1\rangle$$

$$-\ \frac{1}{2}[(N-\ell+2)(M-\ell+4)]^{\frac{1}{2}}\left[\frac{(\ell-m)(\ell+m)(\ell\mp m-1)(\ell\mp m-2)}{(2\ell-3)(2\ell-1)(2\ell-1)(2\ell+1)}\right]^{\frac{1}{2}}|N+2\ \ \ell-2\ \ m\pm1\rangle \tag{IV.88}$$

$$S^{(20)}_{2\pm2}|N\ell m\rangle =$$

$$+ \;[(N-\ell+2)(N+\ell+3)]^{\frac{1}{2}}\left[\frac{(\ell\pm m+1)(\ell\pm m+2)(\ell\mp m)(\ell\pm m-1)}{(2\;\;-1)(2\;\;-1)(2\;\;+3)(2\;\;+3)}\right]^{\frac{1}{2}}|N+2\;\ell\;\;m\pm2\rangle$$

$$+ \left[\frac{(N+\ell+3)(N+\ell+5)}{4}\right]^{\frac{1}{2}}\left[\frac{(\ell\pm m+1)(\ell\pm m+2)(\ell\pm m+3)(\ell\pm m+4)}{(2\ell+1)(2\ell+3)(2\ell+3)(2\ell+5)}\right]^{\frac{1}{2}}|N+2\;\;\ell+2\;\;m\pm2\rangle$$

$$+ \left[\frac{(N-\ell+2)(N-\ell+4)}{4}\right]^{\frac{1}{2}}\left[\frac{(\ell\mp m)(\ell\mp m-1)(\ell\mp m-2)(\ell\mp m-3)}{(2\ell-1)(2\ell-1)(2\ell-3)(2\ell+1)}\right]^{\frac{1}{2}}|N+2\;\;\ell-2\;\;m\pm2\rangle$$

(IV.89)

Finally note that the generators of the Heisenberg group transform as

$$a^{\dagger}_{\pm1} = S^{(10)}_{1\pm1}, \qquad a^{\dagger}_{0} = S^{(10)}_{10}$$
$$a_{\pm1} = S^{(01)}_{1\pm1}, \qquad a_{0} = S^{(01)}_{10} \qquad \text{(IV.90)}$$

VI. <u>Investigation of the Subgroup Structure of $H_4 \times)\, Sp(6,R)$</u>

A more detailed consideration of the subgroup structure of the $H_4 \times)\, Sp(6,R)$ group leads to the group chain $H_4 \times)\, Sp(6,R) \supset Sp(6,R) \supset SU(3) \supset SO(3) \supset SO(2)$. It can be shown that the operators $S^{(NN')}_{LM}$ transform as the (NN') representation of the group SU(3)[43] and the properties of these tensors can be derived using the group chain containing SU(3). Note that the operator $S^{(N'N)}_{L-M}$ transforms contragrediently to the tensor $S^{(NN')}_{LM}$ under the group SU(3).

The study of the tensor product $S^{(N'N)}_{LM} \otimes S^{(N\;N\;)}_{L'M'}$ leads to the consideration of the Kronecker product $(N'N) \times (N\;N\;)$[24]. Take for example $S^{(10)}_{LM} \otimes S^{(10)}_{LM}$. This leads to the Kronecker product $(10) \times (10) = (20) + (01)$ (IV.91)

Now the tensor $S^{(01)}_{LM}$ in this product is completely antisymmetric and so is formed from pairs such as $(a^{\dagger}_{i}a^{\dagger}_{j} - a^{\dagger}_{j}a^{\dagger}_{i})$

Now these are just zero when the boson operator property $[a_i^\dagger a_j^\dagger] = 0$ is used. Hence the products of $a_i^\dagger a_j^\dagger$ all transform as the completely symmetric representation (20) of SU(3).

Similarly $S_{LM}^{(10)} \times S_{LM}^{(01)}$ requires the reduction of

$$(10) \times (01) = (11) + (00) \tag{IV.92}$$

The products $a_i^\dagger a_j$ transform as (11) representations of SU_3 and the symmetric product $a_i^\dagger a_i$ transforms as (00) under SU_3 and is in fact the Hamiltonian of the harmonic oscillator. It is found that the other generators of the $H_4 \times)$ Sp(6,R) may also be constructed using this method.

The construction of the group generators using the SU(3) subgroup chain requires a knowledge of the SU(3) $\supset$ R(3) Clebsch-Gordan coefficients as well as the standard R(3) $\supset$ R(2) Clebsch-Gordan coefficients.

From Vergados the following relations are derived:

$$\langle(\lambda_1\mu_1)k_1L_1M_1|T^{(\mu_2\lambda_2)}_{k_2L_2-m_2}|(\lambda_3\mu_3)k_3L_3M_3\rangle$$
$$= (-i)^\alpha(-1)^{L_2-M_2}\langle(\lambda_3\mu_3)k_3L_3M_3|T^{\lambda_2\mu_2}_{k_2L_2M_2}|(\lambda_1\mu_1)k_1L_1M_1\rangle \tag{IV.93}$$

where $\alpha = 2[\frac{1}{2}(\lambda+L)]$ for $\mu = 0$

$\alpha = 2[\frac{1}{2}(\lambda+L+1)]$ for $\mu = 1$

where $[\lambda]$ is the integral part of x. This relation shows the transformation properties of the contragredient tensor under SU_3. Now following Vergados the following expression for the $H_4 \times)$ Sp(6,R) tensor operators is obtained.

$$\langle(\lambda_3\mu_3)L_3M_3|T^{(\lambda_2\mu_2)}_{L_2M_2}|(\lambda_1\mu_1)L_1M_1\rangle$$
$$= \langle(\lambda_1\mu_2)L_1M_1;(\lambda_2\mu_2)L_2M_2|(\lambda_3\mu_3)L_3M_3\rangle\langle(\lambda_3\mu_3)\,||T^{(\lambda_2\mu_2)}||\,(\lambda_1\mu_1)\rangle \tag{IV.94}$$

which reduces to

$$\langle N_3L_3M_3|T^{(\lambda_2\mu_2)}_{L_2M_2}|N_1L_1M_1\rangle$$

$$= \langle N_1L_1M_1;(\lambda_2\mu_2)L_2M_2|N_3L_3M_3\rangle\langle N_3\,||T^{(\lambda_2\mu_2)}||N_1\rangle \qquad \text{(IV.95)}$$

in the cases being considered.

$\langle N_1L_1M_1;(\lambda_2\mu_2)L_2M_2|N_3L_3M_3\rangle$ is the product of a $SU_3 \supset R_3$ Clebsch-Gordan coefficient and a $R_3 \supset R_2$ Clebsch-Gordan coefficient, while $\langle N_3\,||T^{\lambda_2\mu_2}||N_1\rangle$ is an SU_3 reduced matrix element. The auxiliary quantum number k of equation (IV.93) has been dropped as the representations of SU(3) which are being dealt with reduce to R_3 without the problem of multiple R_3 representations occurring.

For convenience the equation (IV.95) can be factored further into $SU_3 \supset R_3$ and $R_3 \supset R_2$ Clebsch-Gordan coefficients, i.e.

$$\langle N_3L_3M_3|T^{(\lambda\mu)}_{L_2M_2}|N_1L_1M_1\rangle = \langle N_1L_1;(\lambda\mu)L_2||N_3L_3\rangle$$

$$\times \begin{pmatrix} L_1 & L_2 & L_3 \\ M_1 & M_2 & -M_3 \end{pmatrix}\langle N_3\,||T^{(\lambda\mu)}||\,N_1\rangle(-1)^{L_2-L_1-M_3}(2L_3+1)^{\frac{1}{2}},$$

where $\langle N_1L_1;(\lambda\mu)L_2||N_3L_3\rangle$ is a $SU_3 \supset R_3$ Clebsch-Gordan coefficient and $\begin{pmatrix} L_1 & L_2 & L_3 \\ M_1 & M_2 & -M_3 \end{pmatrix}$ is a standard 3-j symbol. A list of the required Clebsch-Gordan coefficients follows. The phase convention here differs from that of Vergados as his corresponds to that of Elliott and the phase convention here is determined by the process of quadruple factorization which determines the phase uniquely. The relationship among different phase conventions of the SU(3) scheme was considered in some detail in chapter two. A list of reduced matrix elements is also given.

Clebsch-Gordan Coefficients taken from Vergados[43] with a Phase Alteration to be Consistent with the rest of this Chapter

$$\langle N_1 L_1;(11)\ell \,\|\, NL\rangle$$

	L_1	
$\ell = 1$	L	$\left[\frac{3L(L+1)}{4N(N+3)}\right]^{\frac{1}{2}}$
$= 2$	$L-2$	$\left[\frac{3(N-L+2)(N+L+1)(L-1)L}{2N(N+3)(2L-1)(2L+1)}\right]^{\frac{1}{2}}$
	L	$-(2N+3)\left[\frac{L(L+1)}{4N(N+3)(2L-1)(2L+3)}\right]^{\frac{1}{2}}$
	$L+2$	$\left[\frac{3(N+L+3)(N-L)(L+2)(L+1)}{2N(N+3)(2L+3)(2L+1)}\right]^{\frac{1}{2}}$

$$\langle N\ L_1;(10)\ell \,\|\, N+1\ L\rangle$$

L_1	
$L-1$	$\left[\frac{(N+L+2)L}{(N+1)(2L+1)}\right]^{\frac{1}{2}}$
$L+1$	$-\left[\frac{(N-L+1)(L+1)}{(N+1)(2L+1)}\right]^{\frac{1}{2}}$

$$\langle N\ L_1;(20)\ell \,\|\, N\ L\rangle$$

	L_1	
$\ell = 0$	L	$\left[\frac{(N-L+2)(N+1+3)}{3(N+1)(N+2)}\right]^{\frac{1}{2}}$
	$L-2$	$\left[\frac{(N+L+1)(N+L+2)(L-1)(L)}{(N+1)(N+2)(2L-1)(2L+1)}\right]^{\frac{1}{2}}$
	L	$-\left[\frac{2(N-L+2)(N+L+3)(L+1)L}{3(N+1)(N+2)(2L-1)(2L+3)}\right]^{\frac{1}{2}}$
	$L+2$	$\left[\frac{(N-L)(N-L+2)(L+2)(L+1)}{(N+1)(N+2)(2L+1)(2L+3)}\right]^{\frac{1}{2}}$

After factorization off of the R_3 Clebsch-Gordan coefficients we get the following relation between Clebsch-Gordan coefficients involving (NO) and (ON) representations of SU_3, viz.

$$\langle N_1L_1;(\lambda_2\mu_2)L_2 \,\|N_3L_3\rangle$$
$$= (-1)^{N_1+\lambda_2-N_3}\langle N_1L_1;(\mu_2\lambda_2)L_2 \,\|N_3L_3\rangle .$$

The corresponding reduced matrix elements are:

$$\langle N \,\|T^{(11)}\|\, N\rangle = [N(N+3)]^{\frac{1}{2}}$$

$$\langle N \,\|T^{(01)}\|\, N+1\rangle = \langle N+1 \,\|T^{(10)}\|\, N\rangle = [N+1]^{\frac{1}{2}}$$

$$\langle N \,\|T^{(02)}\|\, N+2\rangle = \langle N+2 \,\|T^{(20)}\|\, N\rangle = [(N+1)(N+2)]^{\frac{1}{2}}.$$

VII. Construction of the Subgroups of the H_4 ×) Sp(6,R) Group

The group Sp(6,R) contains the following subgroups

The set $S^{(11)}_{LM}$ which generate the group SU(3)

The set $S^{(11)}_{1M}$ which generates the group SO(3)

The set $S^{(11)}_{10}$ which generates the group SO(2)

The set $S^{(20)}_{00}$, $S^{(02)}_{00}$, $S^{(00)}_{00}$ which generate the group O(2,1).

Now consideration of the set of generators of the semi-direct product group

$$H_4 \times)\ S^{(11)}_{LM}, \quad \text{i.e. } (S^{(10)}_{LM}, S^{(01)}_{LM}, E) \times) \{S^{(11)}_{LM}\}$$

generates a group which is closed and has 15 generators since the generators transform as (10) and (01) under SU(3). Following Sen it can be shown that these are just the operators required to extend the SU(3) root figure to the root figure of SU(4) along with an operator which will commute with all of $S_{LM}^{(11)}$. The operator which commutes with all of $S_{LM}^{(11)}$ and is also in H_4 is just the identity E.

Considering the group SU(4) in Cartesian coordinates leads to the general commutation relations

$$[T_{\alpha\beta}\ T_{\gamma\delta}] = T_{\alpha\delta}\delta(\beta\gamma) - T_{\gamma\beta}\delta(\alpha\delta)$$

where $\alpha\beta\gamma\delta$ range over 1,2,3,4. It has already been shown that $T_{\alpha\beta}$, α,β = 1,2,3, generates the group SU(3) and since $T_{\alpha 4}$ and $T_{4\beta}$, α,β = 1,2,3, transform as (10) and (01) under SU(3) respectively, and the operator T_{44} commutes with all of the generators of SU(3), the following identifications are made.

$$\underset{\varepsilon\to 0}{\ell t}\ \varepsilon T_{\alpha 4} = P_{\alpha} \qquad \text{where } P_{\alpha} = a_{\alpha}^{\dagger}$$

$$\underset{\varepsilon\to 0}{\ell t}\ \varepsilon T_{4} = Q_{\beta} \qquad \text{where } Q_{\alpha} = a_{\alpha}$$

$$\underset{\varepsilon\to 0}{\ell t}\ \varepsilon^{2} T_{44} = E.$$

The following sets of commutation relations may be formed:

$$[T_{\alpha\beta}\ T_{\gamma\delta}] = T_{\alpha\delta}\delta(\beta\gamma) - T_{\gamma\beta}\delta(\alpha\delta) \qquad \alpha\beta = 123 \text{ of SU(3)}$$

$$[T_{\alpha\beta}\ T_{\gamma 4}] = T_{\alpha 4}\delta(\beta\gamma) - T_{\gamma\beta}\delta(\alpha 4)$$

$$= T_{\alpha 4} \text{ as } \delta(\alpha 4) = 0 \quad \text{all } \alpha.$$

$$[T_{\alpha\beta}\ T_{4\delta}] = T_{\alpha\delta}\delta(4\beta) - T_{4\beta}\delta(\alpha\delta)$$

$$= -T_{4\beta}\delta(\alpha\delta),$$

and $[T_{\alpha 4}\ T_{4\beta}] = T_{\alpha\beta}\delta(44) - T_{44}\delta(\alpha\beta).$

Now on making the substitutions above, and taking limits

$$[T_{\alpha\beta}\ P_\gamma] = P_\alpha\delta(\beta\gamma)$$

$$[T_{\alpha\beta}\ Q_\gamma] = -Q_\beta\delta(\alpha\gamma)$$

and finally $[P_\alpha\ Q_\beta] = \lim_{\varepsilon\to 0} (\varepsilon^2 T_{\alpha\beta} - \varepsilon^2 T_{44}\delta(\alpha\beta))$

$$= -E\delta(\alpha\beta)$$

with all other commutators being zero. This then introduces the idea that the group $H_4 \times)\ SU(3)$ is a contracted[46,47,48] version of SU(4). But the contraction here is not of the simple Inönü-Wigner type but is of a more complex type dealt with by Saletan[48].

The group chain to be contracted is important and the chain contracted here is

$$SU(n+1) \rightarrow SU(n) \rightarrow R(n) \ldots R(3) \rightarrow R(2)$$

and not the chain

$$SU(n+1) \rightarrow R(n+1) \ldots R(2)$$

where the contracting process carries out the operation

$$SU(n+1) \xrightarrow{\text{contract}} H_{n+1} \times)\ SU(n).$$

This process can be demonstrated diagrammatically as follows:

commutation	SU(3) generators	SU(4) generators
SU(3) generators	SU(3) generators	SU(3) + SU(4) generators
SU(4) generators	SU(3) + SU(4) generators	SU(4) + SU(3) generators

Then after contraction

commutation	SU(3) generators	H_4 generators
SU(3) generators	SU(3) generators	H_4 generators
H_4 generators	H_4 generators	$\begin{matrix} 1 & & 0 \\ & 1 & \\ 0 & & 1 \end{matrix}$

Now a general result can be quoted, that H_{n+1} ×) SU(n) is a contracted version of the group SU(n+1), both groups having n(n+1) generators.

When the group SU(n) is embedded in the group SU(n+1), in the harmonic oscillator basis, two covering groups are required, the group SU(n+1) contains all of the required SU(n) representations up to a fixed number N and all of the rest are in the group SU(n,1). The group proposed here completely covers all of the required SU(n) representations.

It is obvious that the group H_4 ×) SU(3) is non-compact, a consequence of contraction, and completely spans all of the states of the harmonic oscillator. It could be used as a dynamical group for the n dimensional oscillator if one drops the requirement that it contains the transition group O(2,1) × SO(3) as a subgroup. An important point here is that the reduction of the symmetric representation $\{N\}$ of $SU(n+1)$ goes down to $SU(n)$ in the following way

$$\{N\} \rightarrow (N) + (N-1) + (N-2) \ldots (1) + (0)$$

where (N) is a representation of $SU(n)$.

The contracted group is always non-compact because one of the quantum numbers in the parent group is allowed to tend to infinity and means that the contracted group may be formed from a compact parent group. This is useful as the representations of a compact group are usually easier to derive initially than those of its non-compact analogue. This process has one disadvantage in that since similarity transformations do not change the dimension of the representation they cannot be used to obtain infinite-dimensional representations of the contracted group out of the finite dimensional representations of the parent group. Since the contracted group is always non-compact and its unitary representations are infinite dimensional the method cannot be used to derive unitary representations unless the parent group is also non-compact.

The method of constructing these covering groups is given by Hwa and Nuyts[11]. Even in view of all this it seems at present that it may be more difficult to derive the matrix elements of $SU(n+1)$, from $SU(n)$, and then to contract them than it is to construct the matrix elements of $a^{\dagger}_{\pm 1}$, $a_{\pm 1}$, $a^{\dagger}_{0}$, a_0 and build up the required matrix elements directly.

VIII. Other Subgroup Structure in the $H_4 \times) Sp(6,R)$ Group

A study of the groups $H_4 \times) SO(3)$, $H_4 \times) O(2,1)$ leads to the conclusion that $H_4 \times) SO(3)$ is a contracted version of the group O(5) and that $H_4 \times) O(2,1)$ is also a contracted version of O(5). A general result appears at once.

Parent Group	Contracted Group	No. of Generators
$O(2n+2)$	$H_{n+1} \times) Sp(2n,R)$	$(n+1)(2n+1)$
$SU(n+1)$	$H_{n+1} \times) SU(n)$	$n(n+2)$
$O(n+2)$	$H_{n+1} \times) SO(n)$	$\frac{1}{2}(n+2)(n+1)$
$O(n+2)$	$H_{n+1} \times) SO(n-1,1)$	$\frac{1}{2}(n+2)(n+1)$

A more detailed study of these contractions will be the subject of a later work except to remark that the contractions are not of the simple Inönü-Wigner type.

An interesting property that appears for semi-direct products is that if $A \times) B$ is a semidirect product group of A then $A \times) C$ is a subgroup of $A \times) B$ if and only if C is a proper subgroup of B. This is similar to a result which holds for direct products.

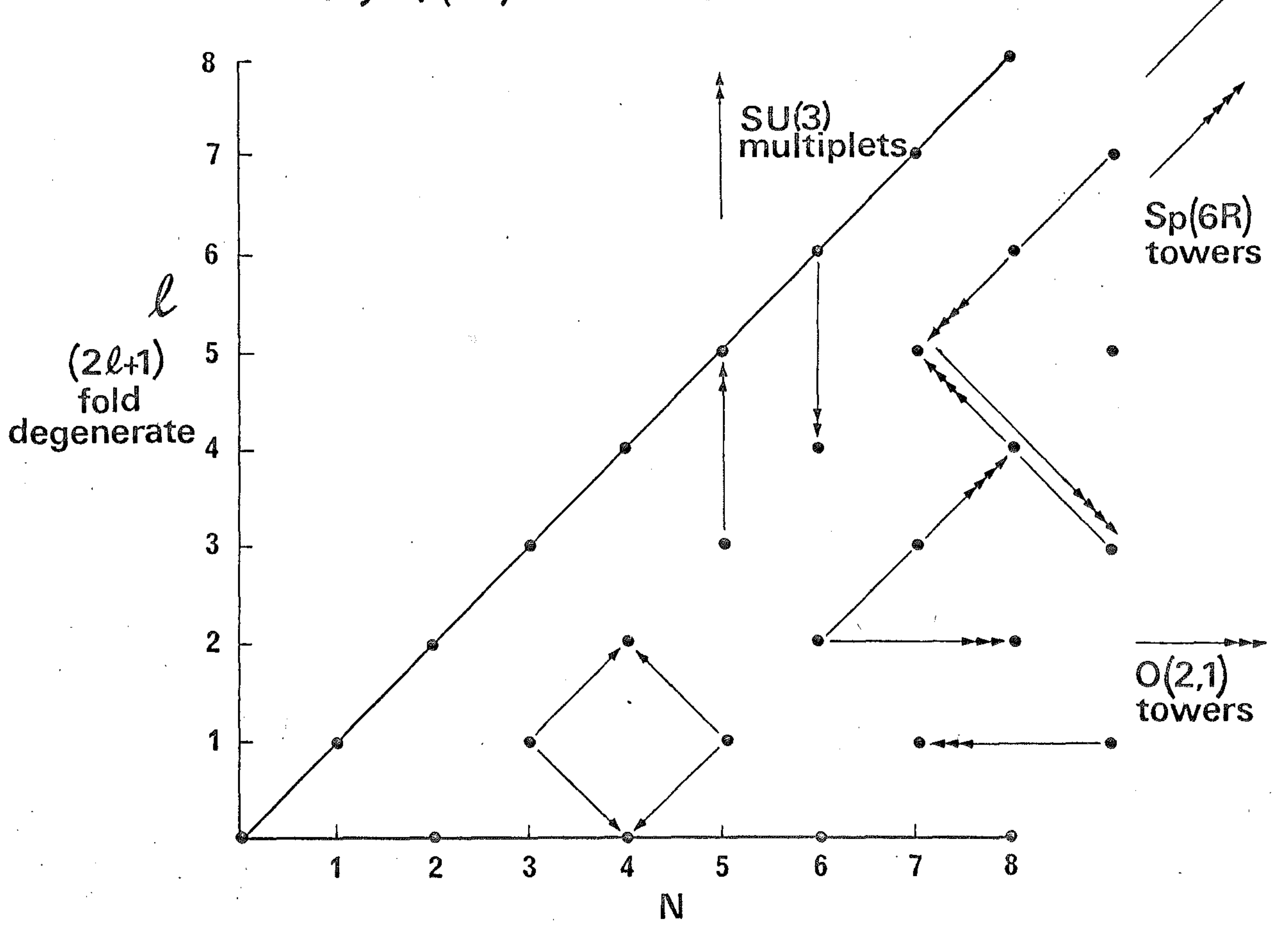
Diagrams showing the properties of the group operators follow.

IX. Some Observations on the One- and Two-Dimensional Oscillators

The states of a two-dimensional harmonic oscillator may be labelled by $|N \rangle$ where N is a $H_3 \times) Sp(4,R)$ quantum number and is the normal R quantum number. The matrix elements of the group generators are:

9 Diagrams of the allowed operations of the group generators

$H_4 \rtimes Sp(6,R)$ 28 parameters

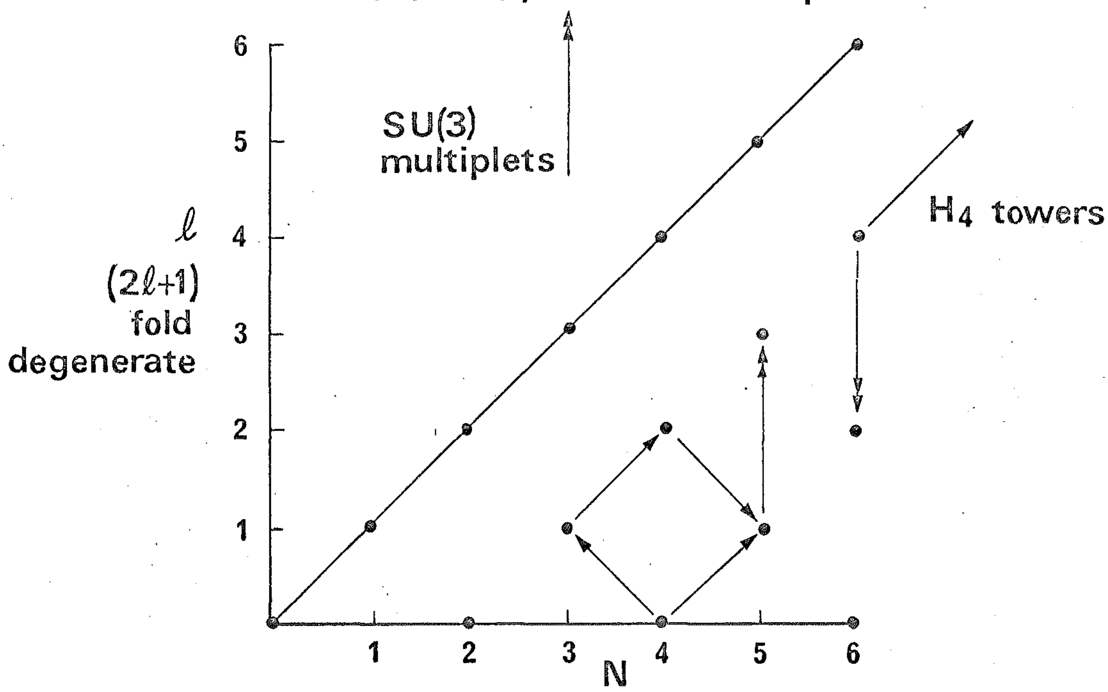


• Denotes an allowed harmonic oscillator state, subject to the condition that $N-\ell$ be even

Group operating	designation
H_4	——►
SU(3)	——►►
O(2,1)	——►►►
Sp(6,R)	——►►►►

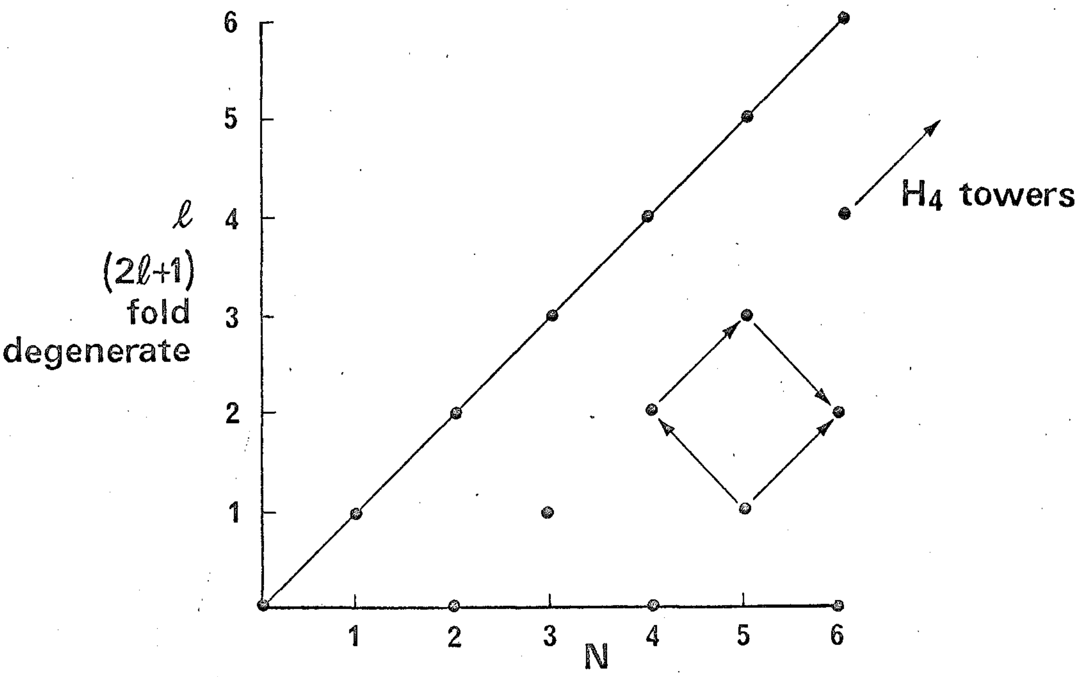
Sub group operations allowed

$H_4 \times) SU(3)$ 15 parameters

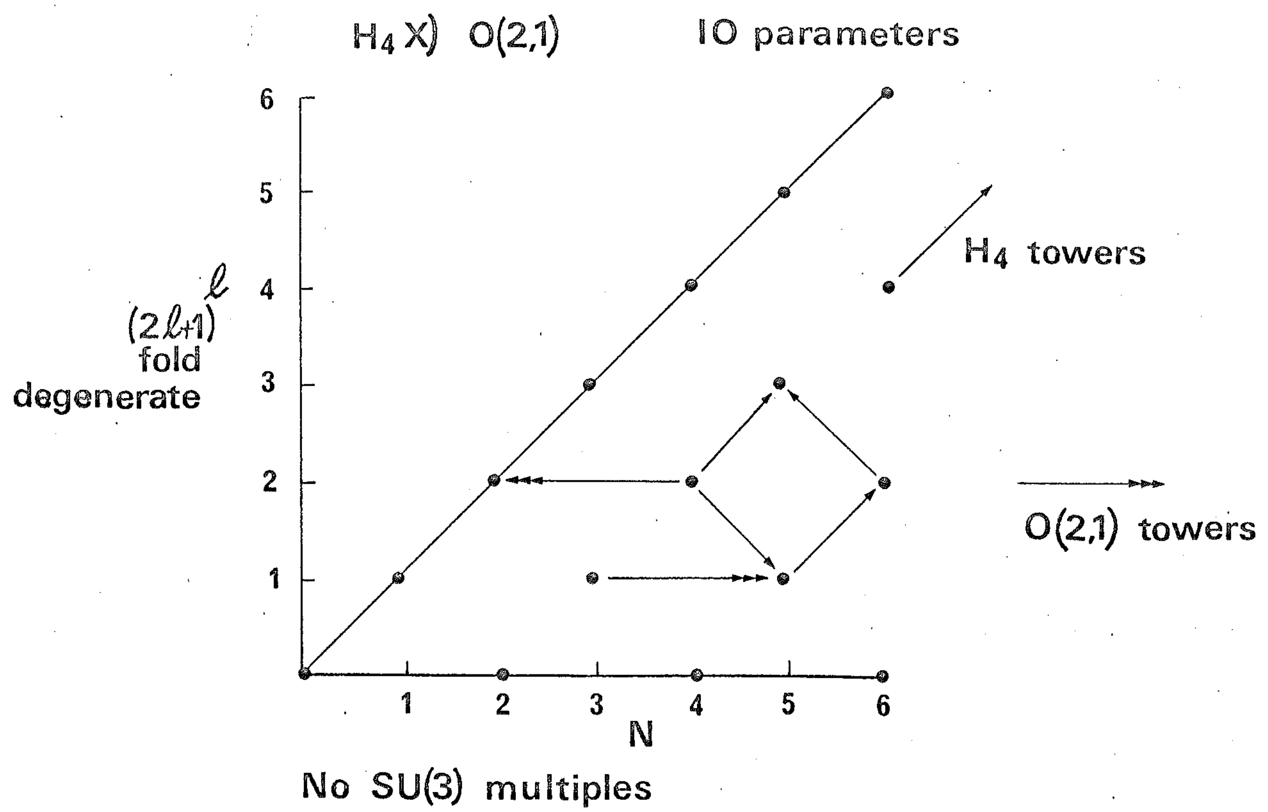


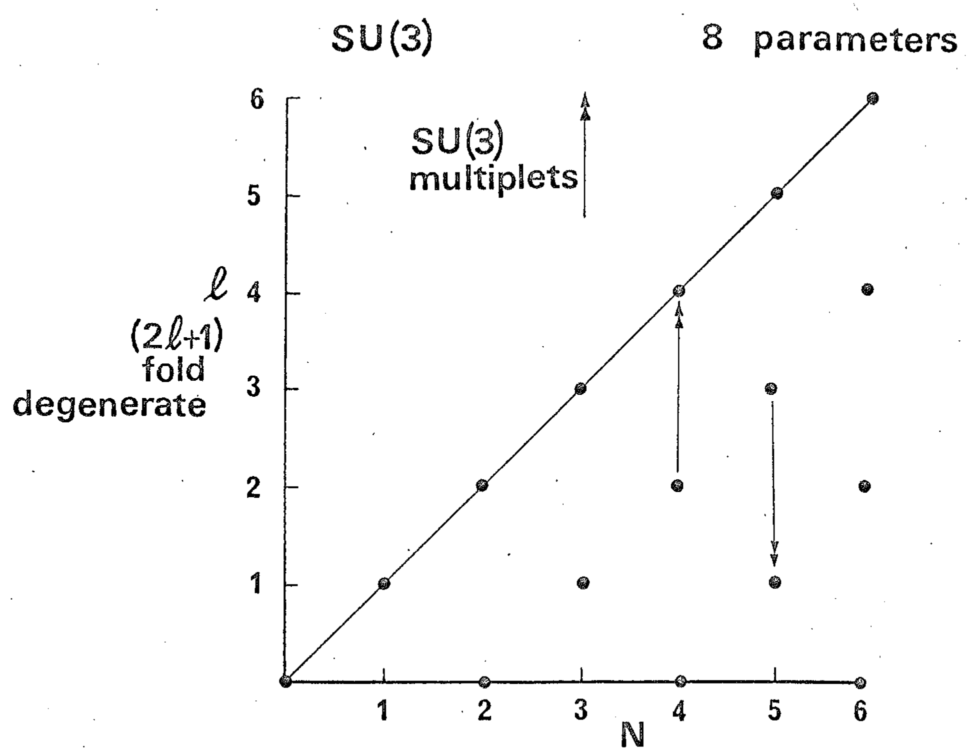
O(2,1) towers are absent

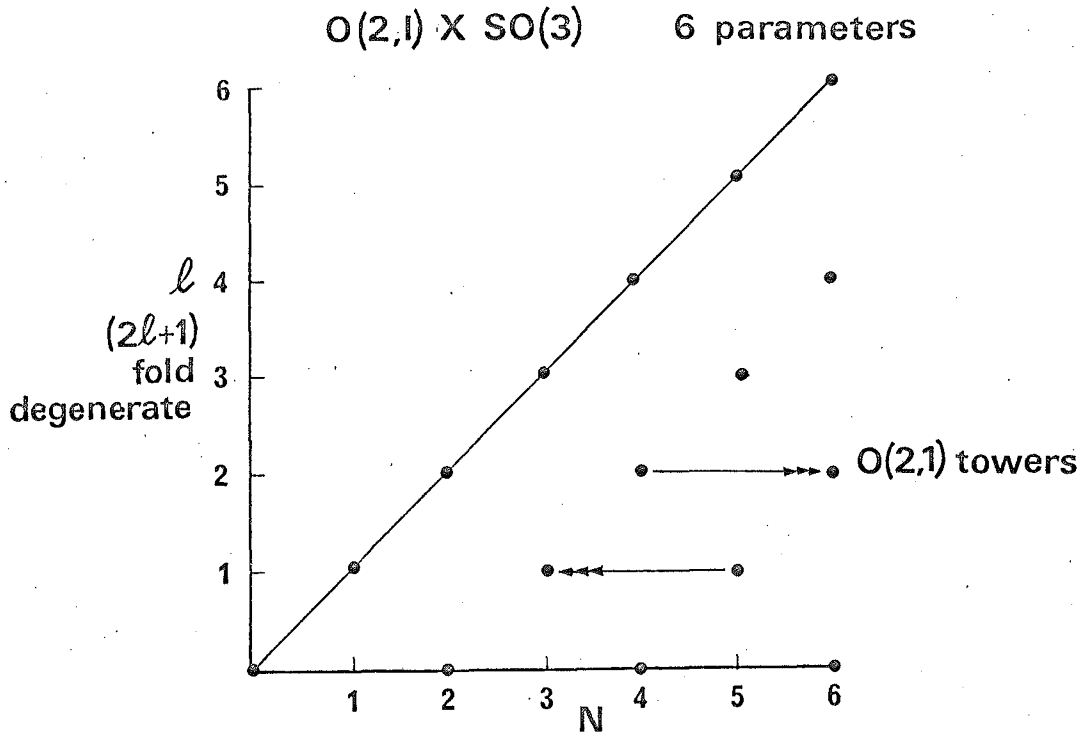
$H_4 \times) SO(3)$ 10 parameters



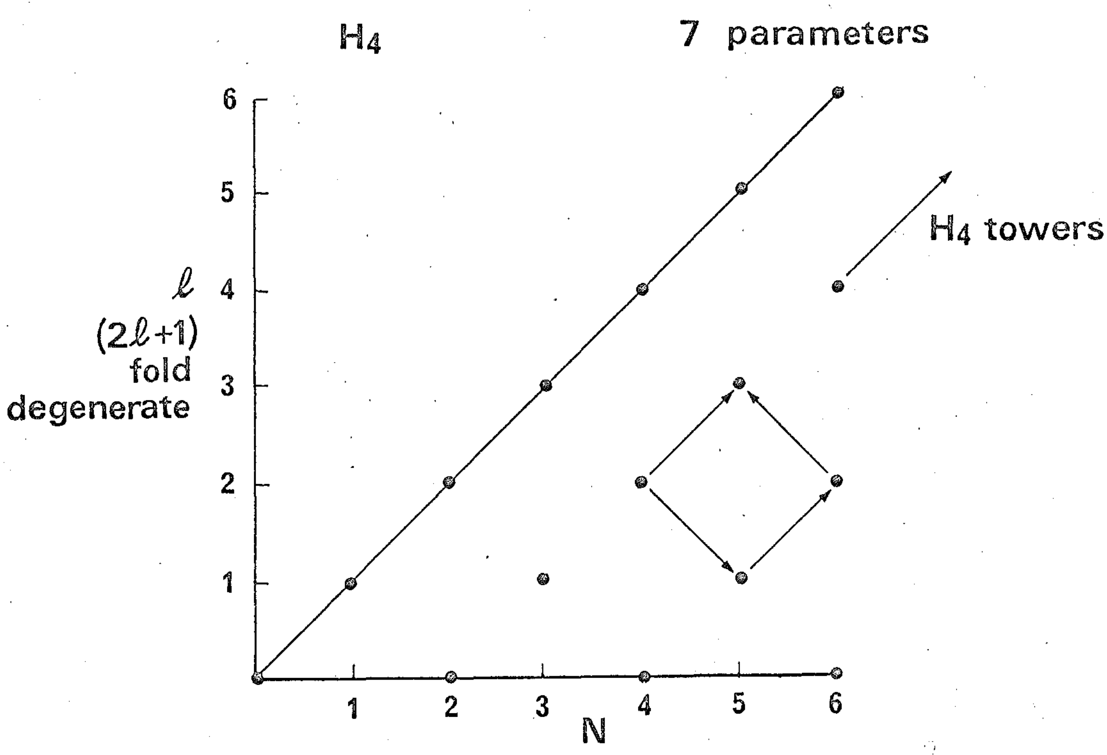
No SU(3) multiplets or O(2,1) towers allowed


H4 X) O(2,1)
10 parameters
6
5
4
3
2
1
ℓ
(2ℓ+1)
fold
degenerate
H4 towers
O(2,1) towers
1
2
3
4
5
6
N
No SU(3) multiples


SU(3)
8 parameters
6
5
4
3
2
1
SU(3)
multiplets
ℓ
(2ℓ+1)
fold
degenerate
1
2
3
4
5
6
N



O(2,1) X SO(3)
6 parameters
ℓ
(2ℓ+1)
fold
degenerate
O(2,1) towers
N



H4
7 parameters
ℓ
(2ℓ+1)
fold
degenerate
H4 towers
N

$$E|Nm\rangle = |Nm\rangle$$

$$a^{\dagger}_{\pm 1}|Nm\rangle = \left[\frac{N\pm m+2}{2}\right]^{\frac{1}{2}}|N+1 \ m\pm 1\rangle$$

$$a_{\pm 1}|Nm\rangle = -\left[\frac{(N\mp m)}{2}\right]^{\frac{1}{2}}|N-1 \ m\pm 1\rangle .$$

For $O(2,1) \times SO(2)$

$$k_0 = \tfrac{1}{2}H|Nm\rangle = \tfrac{1}{2}(N+1) \ |Nm\rangle$$

$$k_+ = -a^{\dagger}_1 a^{\dagger}_{-1}|Nm\rangle$$

$$= -\tfrac{1}{2}[(N-m+2)(N+m+2)]^{\frac{1}{2}}|N+2 \ m\rangle$$

$$k_-|Nm\rangle = -\tfrac{1}{2}[(N+m)(N-m)]^{\frac{1}{2}}|N-2 \ m\rangle$$

$$L_0|Nm\rangle = n|Nm\rangle$$

Remaining generators of $SU(2)$ are

$$Q_{\pm 2}|N\ell m\rangle = \left[\frac{(N\mp m)(N\pm m+2)}{2}\right]^{\frac{1}{2}}|N \ m\pm 2\rangle$$

and the remaining generators of $H_3 \times) \ Sp(4,R)$ are

$$(a^{\dagger}_{\pm 1}a^{\dagger}_{\pm 1})|Nm\rangle = \tfrac{1}{2}[(N\pm m+2)(N\pm m+4)]^{\frac{1}{2}}|N+2 \ m\pm 2\rangle$$

$$(a_{\pm 1}a_{\pm} \ )|Nm\rangle = \tfrac{1}{2}[(N\mp m)(N\mp m-2)]^{\frac{1}{2}}|N-2 \ m\pm 2\rangle .$$

<u>An outline of the group structure present in this case</u>:

		Generators
Dynamical Group	$H_3 \times) \ Sp(4R)$	$L_0, Q_{\pm 2}, k_{\pm}, k_0, a^{\dagger}_{\pm 1}, a_{\pm 1}, E$ $a^{\dagger}_{\pm 1}a^{\dagger}_{\pm 1}$, $a_{\pm 1}a_{\pm 1}$.
Subgroups	$H_3 \times) \ SU(2)$	$L_0, Q_{\pm 2}, a^{\dagger}_{\pm 1}, a_{\pm 1}, E$
	$SU(2)$	L_0, $Q_{\pm 2}$
	$O(2,1) \times SO(2)$	$k_{\pm}, k_0, L_0$
	$SO(2)$	L_0.

The Case of the One-Dimensional Harmonic Oscillator

Dynamical group $H_2 \times) \, Sp(2,R)$

States labelled by $|N\rangle$.

$$O(2,1) \qquad k_0 = \tfrac{1}{2}H|N\rangle = \tfrac{1}{2}(N+\tfrac{1}{2})|N\rangle$$

$$k_+|N\rangle = \tfrac{1}{2}a^\dagger a^\dagger|N\rangle$$

$$= \tfrac{1}{2}[(N+1)(N+2)]^{\frac{1}{2}}|N+2\rangle$$

$$k_-|N\rangle = \tfrac{1}{2}[(N)(N-1)]^{\frac{1}{2}}|N-2\rangle$$

$$a|N\rangle = (N)^{\frac{1}{2}}|N-1\rangle$$

$$a^\dagger|N\rangle = (N+1)^{\frac{1}{2}}|N+1\rangle$$

$$1|N\rangle = |N\rangle.$$

In this case the sumbolism is kept to unify the subject even though some of the groups do not exist.

		Generators
Dynamical Group	$H_2 \times) \, Sp(2,R)$	$a_0^\dagger$, a_0, E, $k_\pm$, k_0
Subgroups	$O(2,1) \times SO(1)$	$k_\pm$, k_0; ——
	SU(1)	——
	SO(1)	——

X. Matrix Elements of H_5 Generators in the Four-Dimensional Harmonic Oscillator

In this case only the matrix elements of the H_5 group are listed as the other group generators may be built up from them in the usual manner. The states of a four-dimensional oscillator are given by

$$|N\ k\ \ell\ m\rangle$$

N is an SU(4) quantum number, R is an R(4) quantum number, ℓ is an R(3) quantum number and m is an R(2) quantum number. The matrix elements of the generators of H_5 are now:

$$a_4^\dagger|Nk\ell m\rangle = -[(N+k+4)]^{\frac{1}{2}}\left[\frac{(k-\ell+1)(k+\ell+1)}{(2k+2)(2k+1)}\right]^{\frac{1}{2}}|N+1\ k+1\ \ell m\rangle$$

$$+\ [N-k+2]^{\frac{1}{2}}\left[\frac{(k-\ell)(k+\ell+1)}{2k(2k+2)}\right]^{\frac{1}{2}}|N+1\ k-1\ \ell m\rangle$$

$$a_4|Nk\ell m\rangle = +\ [N-k]^{\frac{1}{2}}\left[\frac{(k-\ell+1)(k+\ell+2)}{(2k+2)(2k+4)}\right]^{\frac{1}{2}}|N-1\ k+1\ \ell m\rangle$$

$$-\ [N+k+2]^{\frac{1}{2}}\left[\frac{(k-\ell)(k+\ell+1)}{2k(2k+2)}\right]^{\frac{1}{2}}|N-1\ k+1\ \ell m\rangle$$

$$a_0^\dagger|Nk\ell m\rangle = [N+k+4]^{\frac{1}{2}}\left[\frac{(k+\ell+2)(k+\ell+3)(\ell-m+1)(\ell+m+1)}{(2\ell+1)(2\ell+3)(2k+2)(2k+4)}\right]|N+1\ k+1\ \ell+1\ m\rangle$$

$$+\ [N-k+2]^{\frac{1}{2}}\left[\frac{(k-\ell)(k-\ell-1)(\ell-m+1)(\ell+m+1)}{(2\ell+1)(2\ell+3)(2k)(2k+2)}\right]^{\frac{1}{2}}|N+1\ k-1\ \ell+1\ m\rangle$$

$$-\ [(n+k+4)]^{\frac{1}{2}}\left[\frac{(k-\ell+1)(k-\ell+2)(\ell-m)(\ell+m)}{(2\ell-1)(2\ell+1)(2k+1)(2k+4)}\right]^{\frac{1}{2}}|N+1\ k+1\ \ell-1\ m\rangle$$

$$-\ [N-k+2]^{\frac{1}{2}}\left[\frac{(k+\ell)(k+\ell+1)(\ell-m)(\ell+m)}{(2\ell-1)(2\ell+1)(2k)(2k+2)}\right]^{\frac{1}{2}}|N+1\ k-1\ \ell-1\ m\rangle$$

$$a_0|Nk\ell m\rangle = -[N-k]^{\frac{1}{2}}\left[\frac{(k+\ell+2)(k+\ell+3)(\ell-m+1)(\ell+m+1)}{(2\ell+1)(2\ell+3)(2k+2)(2k+4)}\right]^{\frac{1}{2}}|N-1\ k+1\ \ell+1\ m\rangle$$

$$-\ [N+k+2]^{\frac{1}{2}}\left[\frac{(k-\ell)(k-\ell-1)(\ell-m+1)(\ell+m+1)}{(2\ell+1)(2\ell+3)(2k)(2k+2)}\right]^{\frac{1}{2}}|N-1\ k-1\ \ell+1\ m\rangle$$

$$+\ [N-k]^{\frac{1}{2}}\left[\frac{(k-\ell+1)(k-\ell+2)(\ell-m)(\ell+m)}{(2\ell-1)(2\ell+1)(2k+2)(2k+4)}\right]^{\frac{1}{2}}|N-1\ k+1\ \ell-1\ m\rangle$$

$$+\ [N+k+2]^{\frac{1}{2}}\left[\frac{(k+\ell)(k+\ell+1)(\ell-m)(\ell+m)}{(2\ell-1)(2\ell+1)(2k)(2k+2)}\right]^{\frac{1}{2}}|N-1\ k-1\ \ell-1\ m\rangle$$

$$a^{\dagger}_{\pm 1}|Nk\ell m\rangle = +\left[\frac{(n+k+4)}{2}\right]^{\frac{1}{2}}\left[\frac{(k+\ell+2)(k+\ell+3)(\ell\pm m+1)(\ell\pm m+2)}{(2\ell+1)(2\ell+3)(2k+2)(2k+4)}\right]^{\frac{1}{2}}$$

$$|N+1\ \ k+1\ \ \ell+1\ \ m\pm 1\rangle$$

$$+\left[\frac{N-k+2}{2}\right]^{\frac{1}{2}}\left[\frac{(k-\ell)(k-\ell-1)(\ell\pm m+1)(\ell\pm m+2)}{(2\ell+1)(2\ell+3)(2k)(2k+2)}\right]^{\frac{1}{2}}|N+1\ \ k-1\ \ \ell+1\ \ m\pm 1\rangle$$

$$+\left[\frac{N+k+4}{2}\right]^{\frac{1}{2}}\left[\frac{(k-\ell+1)(k-\ell+2)(\ell\mp m)(\ell\mp m-1)}{(2\ell-1)(2\ell+1)(2k+1)(2k+4)}\right]^{\frac{1}{2}}|N+1\ \ k+1\ \ \ell-1\ \ m\pm 1\rangle$$

$$+\left[\frac{N-k+2}{2}\right]^{\frac{1}{2}}\left[\frac{(k+\ell)(k+\ell+1)(\ell\mp m)(\ell\mp m-1)}{(2\ell-1)(2\ell+1)(2k)(2k+2)}\right]^{\frac{1}{2}}|N+1\ \ k-1\ \ \ell-1\ \ m\pm 1\rangle$$

$$a_{\pm 1}|Nk\ell m\rangle = -\left[\frac{(N-k)}{2}\right]^{\frac{1}{2}}\left[\frac{(k+\ell+2)(k+\ell+3)(\ell\pm m+1)(\ell\pm m+2)}{(2\ell+1)(2\ell+3)(2k+2)(2k+4)}\right]^{\frac{1}{2}}$$

$$|N-1\ \ k+1\ \ \ell+1\ \ m\pm 1\rangle$$

$$-\left[\frac{N+k+2}{2}\right]^{\frac{1}{2}}\left[\frac{(k-\ell)(k-\ell-1)(\ell\pm m+1)(\ell\pm m+2)}{(2\ell+1)(2\ell+3)(2k)(2k+2)}\right]^{\frac{1}{2}}|N-1\ \ k-1\ \ \ell+1\ \ m\pm 1\rangle$$

$$-\left[\frac{N-k}{2}\right]^{\frac{1}{2}}\left[\frac{(k-\ell+1)(k-\ell+2)(\ell\mp m)(\ell\mp m-1)}{(2\ell-1)(2\ell+1)(2k+2)(2k+4)}\right]^{\frac{1}{2}}|N-1\ \ k+1\ \ \ell-1\ \ m\pm 1\rangle$$

$$-\left[\frac{N+k+2}{2}\right]^{\frac{1}{2}}\left[\frac{(k+\ell)(k+\ell+1)(\ell\mp m)(\ell\mp m-1)}{(2\ell-1)(2\ell+1)(2k)(2k+2)}\right]^{\frac{1}{2}}|N-1\ \ k-1\ \ \ell-1\ \ m\pm 1\rangle$$

where the first bracket is the $SU(4) \supset SO(4)$ Clebsch-Gordan coefficient, and the second bracket is the product of an $SO(4) \supset SO(3)$ Clebsch-Gordan coefficient and an $SO(3) \supset SO(2)$ Clebsch-Gordan coefficient.

The general scheme of the n-dimensional harmonic oscillator becomes

$n \geqslant 2$

$$H_{n+1} \times) \ Sp(2n,R) \quad \begin{array}{l} Sp(2n,R) \quad (N \text{ even}) \\ Sp(2n,R) \quad (N \text{ odd}) \end{array}$$

$$Sp(2n,R) \quad \begin{array}{l} SO(n) \times O(2,1) \rightarrow SO(3) \times O(2,1) \\ SU(n) \rightarrow SO(n) \rightarrow SO(3) \rightarrow SO(2) \end{array}$$

The other reductions involving semi-direct products are:

$$H_{n+1} \times)\ Sp(2n,R) \rightarrow \begin{cases} H_{n+1} \times)\ \{SO(n) \rightarrow SO(3) \rightarrow SO(2)\} \times O(2,1) \\ H_{n+1} \times)\ \{SU(n) \rightarrow SO(n) \rightarrow SO(3) \rightarrow SO(2)\} \\ \text{all contracted versions of } SU(n+1), \\ \qquad O(n+2) \text{ etc.} \end{cases}$$

XI. Conclusion

In this chapter it has been shown that the group $H_4 \times)\ Sp(6,R)$ spans all of the states of a harmonic oscillator, and is in fact the dynamical group of the three-dimensional harmonic oscillator. The rich subgroup structure has also been investigated and here it becomes obvious that the whole dynamical group is not needed for some specialised calculations (see chapter 3 for examples). Under this scheme the matrix elements of the momentum and position operators may be calculated with ease, and this may be of some considerable use in quantum field theory.

CHAPTER V

GENERAL CONCLUSIONS

In the first two chapters of this thesis it is discovered that the SU(3) scheme is a good approximate symmetry only for the $(d+s)^N$ configurations and that it is no better than the configurational scheme for the $(d+s)^n p^m$ configurations. The SU(3) scheme is found to be an improvement over the configurational scheme in that it makes the calculation of matrix elements easier, due to its well defined symmetry properties. This makes the scheme useful in the calculation of various quantities within the $(d+s)^N$ and $(d+s)^n p^m$ shells of the atoms of the transition series.

The use of the transition group to describe the harmonic oscillator was found to be of considerable use in the calculation of matrix elements of powers of the radial variable r this would make the use of harmonic potentials useful in perturbation theory, especially of molecular systems. The calculations involving harmonic oscillator potentials are easier than those for the hydrogen atom for while there is an infinite number of denumerable states there is no continuum to deal with.

In the last chapter the dynamical group $H_4 \times) Sp(6,R)$ of the three-dimensional oscillator was proposed and its rich subgroup structure investigated. It was seen that the whole dynamical group is not required for some specialized calculations, e.g. the calculation of the matrix elements of r^{2k} where the semi-direct product group $SO(3) \times O(2,1)$ is sufficient. The phase problem which arises with Elliott's[3] derivation of the matrix elements of the SU(3) group generators is eliminated by quadrupole factorization of the harmonic oscillator hamiltonian of Louck[42]. The other great advantage of this group scheme is that the quantities x, y, z, p_x, p_y and p_z are directly expressible in terms of the group generators and this makes the calculation of their matrix elements easier.

Current and future investigations include the use of the semidirect product group in other branches of group theory, a more detailed investigation of the representation theory of semidirect product groups and the contraction of groups to semidirect product groups. Also under investigation at present is the use of the continuous groups in the theory of finite groups, with the view to using them to aid perturbation calculations in ligand field calculations.

APPENDIX I

Definitions of Some Important Terms

1. Commutator Sequence

Iterating the process of forming the commutator group (algebra), one descends along the commutator sequence of the given group (algebra).

2. Contraction

If the infinitesimal operators of a group satisfy the commutation relations $[X_i X_j] = C^k_{ij} X_k$, where C^k_{ij} are the structure constants, and X_i is subject to a linear singular transformation with matrix U, then the new operators Y_i given by $Y_i = U_i{}^j X_j$ form a group with commutation relations $[Y_i Y_j] = C^k_{ij} Y_k$ where C^k_{ij} are the structure constants of the new group. The group $\{Y_i\}$ is then said to be a contraction of the group $\{X_i\}$. See for example Inönü[46,47] and Saletan[48].

3. Degeneracy Group

The degeneracy group of a physical system is the minimal group which has representations that completely span the individual degenerate levels of the system. For example, the levels of the harmonic oscillator are $\frac{(N+1)(N+2)}{2}$ degenerate for a particular N and this is just the dimension of the (NO) representations of SU(3). Note that the matrix elements of its generators cannot couple different degenerate levels.

4. Direct Product

A group G is said to be a direct product of its sub-groups $H_1, H_2 \ldots H_n$ if

i) the elements of different subgroups commute;

ii) every element of G is expressible in one and only one way.

$g = h_1 \ldots h_n$ and it is assumed that none of the subgroups consists of the identity only. Symbolically $G = H_1 \times H_2 \times \ldots \times H_n$.

5. Dynamical Group

The dynamical group is the minimal group containing the degeneracy group and which has a single representation that completely spans all of the allowed levels of the system. For example, in the hydrogen atom O(4,2) is the dynamical group and it contains the degeneracy group SO(4) as well as the transition group $O(2,1) \times SO(3)$. The matrix elements of the dynamical group can couple different degenerate levels.

6. Projective Representation

As this definition takes considerable background to set up, the reader is referred to[49] G.S. Mackey, 'Induced Representations of Groups and Quantum Mechanics' for a full definition.

7. Semi-direct Product

Suppose that a group G has a closed normal subgroup N and that there exists a closed subgroup H of G such that every element X of G may be written uniquely in the form nh, where $n \in N$ and $h \in H$. We may then define a group $N \times) H$ called the semidirect product of N and H with respect to $\times)$ and its elements consist of all pairs n,h where $n \in N$ and $h \in H$ with the multiplication law $(n_1,h_1)(n_2,h_2) = n_1 \times)_{h_1}(n_2)$, h_1h_2, and a straightforward calculation shows all group axioms satisfied[49].

8. Semi-Simple Group

A group is semisimple if none of its non-trivial invariant subgroups are Abelian.

9. Simple Group

A group which has no non-trivial invariant subgroups is said to be simple.

10. Solvable Group

A group (Lie algebra) is said to be solvable if its commutator sequence stops descending after a finite number of steps at $\{1\}(\{0\})$.

11. Transition Group

A transition group is one whose generators couple different degenerate levels of a system, but which does not contain the degeneracy group. For example, in the case of the harmonic oscillator the group O(2,1) couples states with different N values but with the same ℓ value and does not contain the degeneracy group SU(3).

REFERENCES

1. G. Racah, Phys. Rev. 76, 1352 (1949).
   G. Racah, "Group Theory and Spectroscopy", Ergeb. der exakten Naturwiss, Vol. 37 (Springer-Verlag, Berlin, 1965).
2. A.O. Barut and H.M. Kleinert, Phys. Rev. 156, 1541 (1967); Phys. Rev. 157, 1180 (1967); Phys. Rev. 160, 1149 (1967).
3. J.P. Elliott, Proc. Roy. Soc. (London) A245, 128 (1958) Proc. Roy. Soc. (London) A245, 562 (1958) and M. Harvey, Proc. Roy. Soc. A272, 557 (1963).
4. Z.B. Goldschmidt, "Properties and Methods of Interpretation of Rare-Earth Spectra", pp 411-457 in the book, Spectroscopic and Group Theoretical Methods in Physics, edited by F. Bloch, S.G. Cohen, A. de Shalit, S. Sambursky and I. Talmi (North-Holland Publishing Co., Amsterdam, 1968).
5. B.G. Wybourne, "Compact Groups in Atomic Physics", pp 63-121 in book New Directions in Atomic Physics, edited by E.U. Condon and O. Sinanoglu (New Haven and London, Yale University Press, 1972).
6. P.H. Butler and B.G. Wybourne, J. Math. Phys. 11, 2519 (1970).
7. E. Chacón, M. Moshinsky, O. Navaro and C.E. Wulfman, Phys. Rev. A 3, 166 (1971).
8. M. Moshinsky, S. Kumei, T. Shibya and C.E. Wulfman, Istituto de Fisica, in press.

9. L. Armstrong Jr, J. Math. Phys. 12, 953 (1971).
10. M. Moshinsky, T.H. Seligman and K.B. Wolf, J. Math. Phys., in press.
11. C. Quesne and M. Moshinsky, J. Math. Phys. 12, 1780 (1971).
12. R.C. Hwa and J. Nuyts, Phys. Rev. 145, 1188 (1966).
13. A. Crubellier and S. Feneuille, 'Non Compact Groups and the Harmonic Oscillator' in the book The Structure of Matter, edited by B.G. Wybourne (published by University of Canterbury, New Zealand 1972).
14. L.C. Biedenharn and J.D. Louck, Annals of Phys. 63, No.2, 459 (1971).
15. V. Bargmann, Rev. of Modern Phys. 34, No.4, 829 (1962).
16. M.J. Cunningham, Ph.D. Thesis, University of Canterbury (1971).
17. S. Pasternack and R.M. Sternheimer, J. Math. Phys. 3, 1280 (1962).
18. V.A. Fock, Z. Physik 98, 145 (1935).
19. V. Bargmann, Z. Physik 99, 576 (1936).
20. O. Navaro and A. Freyre, Molecular Physics 20, No.5, 861 (1971).
21. G. Racah, Bull. Res. Counc. Israel 3, 290 (1954).
22. M. Moshinsky, The Harmonic Oscillator in Modern Physics: From Atoms to Quarks (Gordon and Breach, New York, 1969).
23. B.R. Judd, Operator Techniques in Atomic Spectroscopy, (McGraw-Hill Book Co., New York, 1963).
24. B.G. Wybourne, Symmetry Principles in Atomic Spectroscopy, (J. Wiley and Sons Inc., New York, 1970).

25. S. Feneuille, J. Physique <u>28</u>, 61 (1967).

26. J.C. Morrison, J. Math. Phys. 10, 1431 (1969).

27. S. Feneuille, J. Physique <u>28</u>, 315 (1967).

28. S. Feneuille, J. Physique <u>28</u>, 701 (1967).

29. P.H. Butler and B.G. Wybourne, J. Physique <u>30</u>, 181 (1969).

30. S. Feneuille, J. Physique <u>30</u>, 325 (1969).

31. S. Feneuille and N. Pelletier-Allard, J. Physique <u>30</u>, 438 (1969).

32. Flores and Moshinsky, Nucl. Phys. <u>A93</u>, 81 (1967).

33. D.E. Littlewood, <u>The Theory of Group Characters</u>, 2nd edition (Oxford University Press, London 1950).

34. Z.B. Goldschmidt and Y. Bordarier, unpublished.

35. L. Armstrong Jr, J. de Phys. (C4) <u>31</u>, 17 (1970).

36. L. Infeld and T.E. Hull, Rev. Mod. Phys. <u>23</u>, 21 (1951).

37. A.O. Barut and E.C. Phillips, Personal Communication.

38. B.L. Van der Waerden, <u>Die Gruppen-theoretische Method in der Quanten Mechanik</u> (Verlag Julius Springer, Berlin, Germany 1932).

39. A.O. Barut and C. Fronsdal, Proc. Roy. Soc. (London) <u>A287</u>, 532 (1965).

40. A.R. Edmonds, <u>Angular Momentum in Quantum Mechanics</u> (Princeton University Press, Princeton 1960).

41. W.H. Shaffer, Rev. Mod. Phys. <u>16</u>, 245 (1944).

42. J.D. Louck and W.H. Shaffer, J. Mol. Spectroscopy <u>4</u>, 285 (1960).

43. J.D. Vergados, Nuclear Physics <u>A111</u>, 681 (1968).

44. R.N. Sen, J. Math. Phys. <u>8</u>, No.4, 896 (1967).

45. M.E. Rose, 'On the Isotropic Harmonic Oscillator', pp 137-152 in the book Spectroscopic and Group Theoretical Methods in Physics, edited by F. Bloch, S.G. Cohen, A. de Shalit, S. Sambursky and I. Talmi (North Holland Publishing Co., Amsterdam 1968).

46. E. Inönü, 'Contraction of Lie Groups and their Representations' in the book Group Theoretical Concepts and Methods in Elementary Particle Physics, edited by F. Gürsey (Gordon and Breach, Science Publishers, London 1962).

47. I. Inönü and E.P. Wigner, Proc. Nat. Acad. 39, 510 (1953).

48. E.J. Saletan, J. Math. Phys. 2, No. 1, 1 (1961).

49. G.W. Mackey, Induced Representations of Groups and Quantum Mechanics, (W.A. Benjamin, Inc., New York 1968).

50. W.J. Holman and L.C. Biedenharn, Annals of Phys. 39, 1 (1966).

PUBLICATIONS

A large part of this thesis has either been published or submitted for publication. In detail:

Chapter 1: 'Application of the Group SU(3) to the Theory of the Many-Electron Atom', Physica 53, 64 (1971).

Chapter 2: 'Etude des configurations $(d+s)^n p^m$ au moyen du group SU(3)', J. de Physique colloque C4, supplement au n° 11-12, Tome 31, Nov-Dec. 1970, page C4-25.

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